Microfluidics Module

User's Guide

6.3

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Microfluidics Module User's Guide

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1

Introduction

This guide describes the Microfluidics Module, an optional add-on package that extends the COMSOL Multiphysics® modeling environment with customized physics interfaces for microfluidics.

This chapter introduces you to the capabilities of this module. A summary of the physics interfaces and where you can find documentation and model examples is also included. The last section is a brief overview with links to each chapter in this guide.

In this chapter:

- About the Microfluidics Module
- Overview of the User's Guide

About the Microfluidics Module

In this section:

- About Microfluidics
- About the Microfluidics Module
- The Microfluidics Module Physics Interface Guide
- Coupling to Other Physics Interfaces
- The Microfluidics Module Study Capabilities by Physics Interface
- Common Physics Interface and Feature Settings and Nodes
- The Liquids and Gases Materials Database
- Where Do I Access the Documentation and Application Libraries?

About Microfluidics

The field of ***microfluidics*** evolved as engineers and scientists explored new avenues to make use of the fabrication technologies developed by the microelectronics industry. These technologies enabled complex micron and submicron structures to be integrated with electronic systems and batch fabricated at low cost. Mechanical devices fabricated using these technologies have become known as microelectromechanical systems (MEMS), whilst fluidic devices are commonly referred to as microfluidic systems or "lab-on-a-chip" devices. A proper description of these microsystems usually requires multiple physical effects to be incorporated.

At the microscale different physical effects become important to those dominant at macroscopic scales. Properties that scale with the volume of the system (such as inertia) become comparatively less important than those that scale with the surface area of the system (such as viscosity and surface tension). Fluid flow is therefore usually laminar and chemical migration is often limited by diffusion. Electrokinetic effects become important as the electric double layers present at interfaces in the system interact with external applied fields. As systems are further miniaturized, the mean free path of the fluid can become comparable to the size of the system and rarefaction effects become important. At moderate Knudsen numbers (the Knudsen number is the ratio of the mean free path to the system size), it is still possible to use the Navier-Stokes equations to solve the flow; however, special slip boundary conditions are required.

Research activity in microfluidics is changing medical-diagnostic processes such as DNA analysis, and it is spurring the development of successful commercial products.

Tools to address the flow of fluids within porous media are also included as well as a physics interface to model moderately rarefied gas flows (the Slip Flow interface).

About the Microfluidics Module

The Microfluidics Module is a collection of tailored physics interfaces for the simulation of microfluidic devices. It has a range of tools to address the specific challenges of modeling micro- and nanoscale flows.

Physics interfaces that address laminar flow, multiphase flow, flow in porous media, and moderately rarefied flow (the Slip Flow interface) are available. Enhanced capabilities to treat chemical reactions between dilute species are also included. COMSOL Multiphysics also has tools to model the transport and reactions of concentrated species, but the Chemical Reaction Engineering Module is required for these physics interfaces. In addition to the standard tools for modeling fluid flow, interfaces between fluids can be modeled by the Level Set, Phase Field in Fluids, and Moving Mesh interfaces, making it possible to model surface tension and multiphase flow at the microscale.

The Microfluidics Module Application Library and supporting documentation explain how to use the physics interfaces to model a range of microfluidic devices.

The Microfluidics Module Physics Interface Guide

The physics interfaces in the Microfluidics Module form a complete set of simulation tools, which extends the functionality of the physics interfaces of the base package for COMSOL Multiphysics. The details of the physics interfaces and study types for the Microfluidics Module are listed in the table. The functionality of the COMSOL Multiphysics base package is given in the *COMSOL Multiphysics Reference Manual*.

	In the *COMSOL Multiphysics Reference Manual:* • Studies and Solvers • The Physics Interfaces • For a list of all the core physics interfaces included with a COMSOL Multiphysics license, see Physics Interface Guide.

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Chemical Species Transport				
Transport of Diluted Species[1]		tds	all dimensions	stationary; time dependent
Transport of Diluted Species in Porous Media		tds	all dimensions	stationary; time dependent
Reacting Flow				
Laminar Flow, Diluted Species[1]		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Fluid Flow				
Single-Phase Flow				
Creeping Flow		spf	3D, 2D, 2D axisymmetric	stationary; time dependent
Laminar Flow[1]		spf	3D, 2D, 2D axisymmetric	stationary; time dependent
Potential Flow				
Incompressible Potential Flow		ipf	3D, 2D, 2D axisymmetric	stationary
Multiphase Flow				
Two-Phase Flow, Moving Mesh				
Laminar Two-Phase Flow, Moving Mesh		—	3D, 2D, 2D axisymmetric	time dependent
Two-Phase Flow, Level Set				
Laminar Two-Phase Flow, Level Set		—	3D, 2D, 2D axisymmetric	time dependent with phase initialization

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Two-Phase Flow, Phase Field				
Laminar Two-Phase Flow, Phase Field		—	3D, 2D, 2D axisymmetric	time dependent with phase initialization
Three-Phase Flow, Phase Field				
Laminar, Three-Phase Flow, Phase Field		—	3D, 2D, 2D axisymmetric	time dependent with phase initialization
Porous Media and Subsurface Flow				
Brinkman Equations		br	3D, 2D, 2D axisymmetric	stationary; time dependent
Darcy's Law		dl	all dimensions	stationary; time dependent
Free and Porous Media Flow, Brinkman		fp	3D, 2D, 2D axisymmetric	stationary; time dependent
Free and Porous Media Flow, Darcy		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Fluid-Structure Interaction				
Fluid–Solid Interaction, Fixed Geometry[2]		—	3D, 2D, 2D axisymmetric	stationary; stationary, one way; time dependent; time dependent, one way
Fluid–Solid Interaction, Two-Phase Flow, Phase Field, Fixed Geometry[2]		—	3D, 2D, 2D axisymmetric	time dependent; time dependent with phase initialization
Rarefied Flow				
Slip Flow		slpf	3D, 2D, 2D axisymmetric	stationary; time dependent

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Mathematics				
Moving Interface				
Level Set		ls	all dimensions	time dependent with phase initialization
Level Set in Porous Media		ls	all dimensions	time dependent with phase initialization
Phase Field in Fluids		pf	all dimensions	time dependent; time dependent with phase initialization
Ternary Phase Field		terpf	3D, 2D, 2D axisymmetric	time dependent

[1] This physics interface is included with the core COMSOL Multiphysics software but has added functionality for this module.

Coupling to Other Physics Interfaces

The Microfluidics Module connects to COMSOL Multiphysics and other add-on modules in the COMSOL Multiphysics product line. Table 1-1 summarizes the most important microfluidics couplings and other common devices you can model.

The *Microfluidics* column lists transport phenomena that are key issues in, for example, lab-on-a-chip type devices.

This list is only the tip of the iceberg — an overview of the most important applications where you can use the Microfluidics Module. In your hands, the multiphysics combinations and applications are unlimited.

TABLE 1-1: EXAMPLES OF COUPLED PHENOMENA AND DEVICES YOU CAN MODEL USING THE MICROFLUIDICS MODULE.

	MICROFLUIDICS
PHENOMENA/ COUPLING	Pressure-driven flow
	Chemical Reactions in two-phase flow
	Dielectrophoresis
	Electroosmotic flow
	Electrophoresis
	Electrothermal flow
	Electrowetting
	Fluid-Structure interaction
	Magnetophoresis
	Mass transport using diffusion, migration, and convection
	Slip Flow
DEVICES	Lab-on-a-chip devices
	Microfluidic channels
	Microreactors
	Micromixers
	MEMS heat exchangers
	Nonmechanical pumps and valves

The Microfluidics Module Study Capabilities by Physics Interface

Table 1-2 lists the Preset Studies available for each physics interface specific to this module.

When using the axisymmetric interfaces, the horizontal axis represents the r direction and the vertical axis the z direction. The geometry must be created in the right half plane (that is, only for positive r).

Studies and Solvers in the *COMSOL Multiphysics Reference Manual*

TABLE 1-2: MICROFLUIDICS MODULE DEPENDENT VARIABLES AND PRESET STUDY AVAILABILITY.

PHYSICS INTERFACE	NAME	DEPENDENT VARIABLES	PRESET STUDIES*		
			STATIONARY	TIME DEPENDENT	TRANSIENT WITH INITIALIZATION
CHEMICAL SPECIES TRANSPORT					
Transport of Diluted Species	tds	c	√	√	
Transport of Diluted Species in Porous Media	tds	c	√	√	
FLUID FLOW>RAREFIED FLOW					
Slip Flow	slpf	u, v, w, p, T	√	√	
FLUID FLOW>SINGLE-PHASE FLOW					
Laminar Flow	spf	u, v, w, p	√	√	
Creeping Flow	spf	u, v, w, p	√	√	
Incompressible Potential Flow	ipf	ϕ	√		
FLUID FLOW>MULTIPHASE FLOW					
Laminar Two-Phase Flow, Level Set	tpf	u, v, w, p, ϕ			√
Laminar Two-Phase Flow, Phase Field	tpf	u, v, w, p, ϕ, ψ			√
Laminar Two-Phase Flow, Moving Mesh	spf	u, v, w, p		√	
Laminar Three-Phase Flow, Phase Field	tfpf	u, v, w, p, ϕ, η		√	
FLUID FLOW>POROUS MEDIA AND SUBSURFACE FLOW					
Brinkman Equations	br	u, v, w, p	√	√	
Darcy's Law	dl	p	√	√	
Free and Porous Media Flow, Brinkman	fp	u, v, w, p	√	√	
Free and Porous Media Flow, Darcy	-	u, v, w, p	√	√	
MATHEMATICS					
Level Set	ls	ϕ			√
Phase Field in Fluids	pf	ϕ, ψ			√

TABLE 1-2: MICROFLUIDICS MODULE DEPENDENT VARIABLES AND PRESET STUDY AVAILABILITY.

PHYSICS INTERFACE	NAME	DEPENDENT VARIABLES	PRESET STUDIES*		
			STATIONARY	TIME DEPENDENT	TRANSIENT WITH INITIALIZATION
Ternary Phase Field	terpf	ϕ, η		√	
Custom studies are also available based on the physics interface.					

Common Physics Interface and Feature Settings and Nodes

There are several common settings and sections available for the physics interfaces and feature nodes. Some of these sections also have similar settings or are implemented in the same way no matter the physics interface or feature being used. There are also some physics feature nodes that display similarities in COMSOL Multiphysics.

In each module's documentation, only unique or extra information is included; standard information and procedures are centralized in the *COMSOL Multiphysics Reference Manual*.

!	In the *COMSOL Multiphysics Reference Manual* see Table 2-4 for links to common sections and Table 2-5 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

The Liquids and Gases Materials Database

The Microfluidics Module includes an additional **Liquids and Gases** material database with temperature-dependent fluid dynamic and thermal properties.

For detailed information about materials and the Liquids and Gases Material Library, see Materials in the *COMSOL Multiphysics Reference Manual*.

Where Do I Access the Documentation and Application Libraries?

A number of online resources have more information about COMSOL, including licensing and technical information. The electronic documentation, topic-based (or context-based) help, and the Application Libraries are all accessed through the COMSOL Desktop.

If you are reading the documentation as a PDF file on your computer, the blue links do not work to open an application or content referenced in a different guide. However, if you are using the Help system in COMSOL Multiphysics, these links work to open other modules, application examples, and documentation sets.

THE DOCUMENTATION AND ONLINE HELP

The *COMSOL Multiphysics Reference Manual* describes the core physics interfaces and functionality included with the COMSOL Multiphysics license. This book also has instructions on how to use COMSOL Multiphysics and how to access the electronic Documentation and Help content.

Opening Topic-Based Help

The Help window is useful as it is connected to the features in the COMSOL Desktop. To learn more about a node in the Model Builder, or a window on the Desktop, click to highlight a node or window, then press F1 to open the Help window, which then

displays information about that feature (or click a node in the Model Builder followed by the **Help** button (?). This is called *topic-based* (or *context) help*.

Win	To open the **Help** window: • In the **Model Builder**, **Application Builder**, or **Physics Builder**, click a node or window and then press F1. • On any toolbar (for example, **Home**, **Definitions**, or **Geometry**), hover the mouse over a button (for example, **Add Physics** or **Build All**) and then press F1. • From the **File** menu, click **Help** (?). • In the upper-right corner of the COMSOL Desktop, click the **Help** (?) button.

Mac Linux	To open the **Help** window: • In the **Model Builder** or **Physics Builder**, click a node or window and then press F1. • In the main toolbar, click the **Help** (?) button. • From the main menu, select **Help>Help**.

Opening the Documentation Window

Mac Linux	To open the **Documentation** window: • Press Ctrl+F1. • In the main toolbar, click the **Documentation** ( ) button. • From the main menu, select **Help>Documentation**.

THE APPLICATION LIBRARIES WINDOW

Each model or application includes documentation with the theoretical background and step-by-step instructions to create a model or application. The models and applications are available in COMSOL Multiphysics as MPH-files that you can open for further investigation. You can use the step-by-step instructions and the actual models as templates for your own modeling. In most models, SI units are used to describe the relevant properties, parameters, and dimensions, but other unit systems are available.

Once the Application Libraries window is opened, you can search by name or browse under a module folder name. Click to view a summary of the model or application and its properties, including options to open it or its associated PDF document.

Opening the Application Libraries Window

To open the **Application Libraries** window ( ):

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To receive technical support from COMSOL for the COMSOL products, please contact your local COMSOL representative or send your questions to support@comsol.com. An automatic notification and a case number will be sent to you by email. You can also access technical support, software updates, license information, and other resources by registering for a COMSOL Access account.

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Support Knowledge Base	www.comsol.com/support/knowledgebase

Overview of the User's Guide

The *Microfluidics Module User's Guide* gets you started with modeling microfluidic systems using COMSOL Multiphysics. The information in this guide is specific to this module. Instructions how to use COMSOL Multiphysics in general are included with the *COMSOL Multiphysics Reference Manual*.

	As detailed in the section Where Do I Access the Documentation and Application Libraries? this information can also be searched from the COMSOL Multiphysics software **Help** menu.

TABLE OF CONTENTS, GLOSSARY, AND INDEX

To help you navigate through this guide, see the Contents, Glossary, and Index.

MODELING IN MICROFLUIDICS

The Microfluidic Modeling chapter familiarizes you with modeling procedures useful when working with this module. Topics include Physics and Scaling in Microfluidics, Dimensionless Numbers in Microfluidics, Modeling Microfluidic Fluid Flows, Modeling Coupled Phenomena in Microfluidics, and Modeling Rarefied Gas Flows.

THE FLUID FLOW BRANCH INTERFACES

There are several fluid flow interfaces available. The various types of momentum transport that you can simulate include laminar and creeping flow, multiphase two-phase flow, and flow in porous media. Every section describes the applicable physics interfaces in detail and concludes with the underlying interface theory.

Single-Phase Flow

Single-Phase Flow Interfaces chapter describes the Laminar Flow, Creeping Flow and Incompressible Potential Flow interfaces.

Multiphase Flow Two-Phase Flow

Multiphase Flow, Two-Phase Flow Interfaces chapter describes the Laminar Two-Phase Flow Level Set and Phase Field interfaces, as well as the Laminar Three-Phase Flow, Phase Field and the Laminar Two-Phase Flow, Moving Mesh interface. Some multiphase flow is described using the Phase Field in Fluids, Level Set, and Ternary Phase Field interfaces found under Mathematics, Moving Interfaces

branch. In this module, these physics are already integrated into the relevant physics interfaces.

Porous Media and Subsurface Flow

Porous Media Flow Interfaces chapter describes the Darcy's Law, Brinkman Equations, and Free and Porous Media Flow interfaces.

Rarefied Flow

Rarefied Flow Interface chapter describes the Slip Flow interface, including the underlying theory.

THE CHEMICAL SPECIES TRANSPORT BRANCH INTERFACES

The transport and conversion of material is denoted as chemical species transport. Chemical Species Transport Interfaces chapter describes the Transport of Diluted Species and the Transport of Diluted Species in Porous Media as well as the underlying theory.

2

Microfluidic Modeling

This chapter gives an overview of the physics interfaces available for modeling microfluidic flows and provides guidance on choosing the appropriate physics interface for a specific problem.

In this chapter:

- Physics and Scaling in Microfluidics
- Dimensionless Numbers in Microfluidics
- Modeling Microfluidic Fluid Flows
- Modeling Coupled Phenomena in Microfluidics
- Modeling Rarefied Gas Flows

Physics and Scaling in Microfluidics

Microfluidic flows occur on length scales that are orders of magnitude smaller than macroscopic flows. Manipulation of fluids at the microscale has a number of advantages — typically microfluidic systems are smaller, operate faster, and require less fluid than their macroscopic equivalents. Energy inputs and outputs are also easier to control (for example, heat generated in a chemical reaction) because the surface-to-area volume ratio of the system is much greater than that of a macroscopic system.

In general, as the length scale (L) of the fluid flow is reduced, properties that scale with the surface area of the system become comparatively more important than those that scale with the volume of the flow (see Table 2-1). This is apparent in the fluid flow itself as the viscous forces, which are generated by shear over the isovelocity surfaces (scaling as L^2), dominate over the inertial forces (which scale volumetrically as L^3). The Reynolds number (Re), which characterizes the ratio of these two forces, is typically low, so the flow is laminar. In many cases the creeping (Stokes) flow regime applies ($\mathrm{Re} \ll 1$). The section Single-Phase Flow describes microfluidic fluid flows in greater detail.

When multiple phases are present surface tension effects become important relative to gravity and inertia at small length scales. The Laplace pressure, capillary force, and Marangoni forces all scale as $1/L$. The section Multiphase Flow gives more information on modeling flows involving several phases.

Flow through porous media can also occur on microscale geometries. Because the permeability of a porous media scales as L^2 (where L is the average pore radius) the flow is often friction dominated when the pore size is in the micron range and Darcy's law can be used. For intermediate flows this module also provides a physics interface to model flows where Brinkman equation is appropriate. For more information see Porous Media Flow.

At the microscale, a range of electrohydrodynamic effects can be used to influence the fluid flow. The electric field strength for a given applied voltage scales as $1/L$, making it easier to apply relatively large fields to the fluid with moderate voltages. In electroosmosis the uncompensated ions in the charged electric double layer (EDL) present on the fluid surfaces are moved by an electric field, causing a net fluid flow. Electrophoretic and dielectrophoretic forces on charged or polarized particles in the fluid can be used to induce particle motion, as can diamagnetic forces in the case of

magnetophoresis. The manipulation of contact angles by the electrowetting phenomena is also easy in microscale devices. The section Electrohydrodynamics explains how to model these phenomena in detail.

TABLE 2-1: SCALING OF VARIOUS PHYSICAL PHENOMENA WITH LENGTH (L) AND THE CONSEQUENCES FOR MICROFLUIDIC DEVICES.

PROPERTY	LENGTH SCALING	CONSEQUENCES
Volume	L^3	Surface related properties increase in importance relative to volumetric properties, Surface area to volume ratios are high.
Area	L^2	
Inertial Forces	L^3	Viscosity dominates over inertia, flow is laminar or creeping. Absence of convection makes mixing difficult.
Viscous Forces	L^2	
Laplace Pressure	L^{-1}	Surface tension effects become dominant in two phase flows.
Capillary Force	L^{-1}	
Permeability of Porous media	L^2	Darcy's law usually applies.
Diffusion Time Scale	L^2	Diffusive mixing possible (although still much slower than convection).
Electric Field (at constant applied voltage)	L^{-1}	Possibility of using a range of electrokinetic effects to drive the flow.
Knudsen Number	L^{-1}	Microscale gas flows are usually rarefied.

Laminar flows make mixing particularly difficult, so mass transport is often diffusion limited. The diffusion time scales as L^2, but even in microfluidic systems diffusion is often a slow process. This has implications for chemical transport and hence reactions within microfluidic systems. Chemical Transport and Reactions describes how to model diffusion-based transport and chemical reactions in microfluidics.

As the length scale of the flow becomes comparable to intermolecular length scale, more complex kinetic effects become important. For gases the ratio of the molecular mean free path to the flow geometry size is given by the Knudsen number (Kn). Clearly, Kn scales as $1/L$. For $\mathrm{Kn} < 0.01$, fluid flow is usually well described by the Navier–Stokes equations with no-slip boundary conditions. In the slip flow regime ($0.01 < \mathrm{Kn} < 0.1$) appropriate slip boundary conditions can be used with the Navier-Stokes equations to describe the flow away from the boundary (see Slip Flow). At Knudsen numbers above 0.1 a fully kinetic approach is required. Flows in this regime can be modeled using tools from the Molecular Flow Module.

The next section describes the importance of Dimensionless Numbers in Microfluidics, which are frequently used in transport equations.

	The Free Molecular Flow and Transitional Flow interfaces are available in the Molecular Flow Module.

	The Physics Interfaces and Building a COMSOL Multiphysics Model in the *COMSOL Multiphysics Reference Manual*

Dimensionless Numbers in Microfluidics

Information about the dominant physics in a microfluidics problem is contained in many of the dimensionless numbers that are used to characterize the flow. When using the finite element method, dimensionless numbers defined on the element or "cell" level can contain important information about the numerical stability of the problem (the term "cell" is carried over from the finite volume method in this context). This section includes information about the dimensionless numbers that are relevant to microfluidic flows.

In this section:

- Dimensionless Numbers Important for Solver Stability
- Other Dimensionless Numbers

Dimensionless Numbers Important for Solver Stability

When solving a microfluidics problem numerically there are two critical dimensionless numbers to consider in terms of solver stability. These numbers are:

- The Reynolds number (Re)
- The Peclet number (Pe)

Each of these numbers is defined in Table 2-2. Both the Reynolds number and the Peclet number are associated with the relative importance of convective terms in the corresponding partial differential equation. The *Peclet number* describes the importance of convection in relation to diffusion (for either heat or mass transfer), and the *Reynolds number* describes the importance of the "convective" inertia term in relation to viscosity in the Navier–Stokes equations themselves.

Both the Reynolds number and the Peclet number can be defined on the "cell" or element level. As they are defined in COMSOL Multiphysics numerical instabilities can arise when the cell Reynolds or Peclet number is greater than one. These instabilities are usually manifested as spurious oscillations in the solution. Taking the Peclet

number as an example, oscillations can occur when the cell Peclet number is greater than one in the following circumstances:

- A Dirichlet boundary condition can lead to a solution containing a steep gradient near the boundary, forming a boundary layer. If the mesh cannot resolve the boundary layer, this creates a local disturbance.
- A space-dependent initial condition that the mesh does not resolve can cause a local initial disturbance that propagates through the computational domain.
- A small initial diffusion term close to a nonconstant source term or a nonconstant Dirichlet boundary condition can result in a local disturbance.

In theory the grid can be refined to bring the cell Reynolds or Peclet number below one, although this is often impractical for many problems. Several stabilization techniques are included, which enable problems with larger cell Reynolds or Peclet numbers to be solved. At the crudest level additional numerical diffusion can be added to the problem to improve its stability. This is achieved by selecting **Isotropic Diffusion** under **Inconsistent Stabilization** for any physics interface.

	The stabilization options are visible when the **Show More Options** button ( ) is clicked and **Stabilization** is selected in the **Show More Options** dialog.

This method is termed "inconsistent" as a solution to the problem without numerical diffusion is not necessarily a solution to the problem with diffusion. COMSOL Multiphysics also has consistent stabilization options. A consistent stabilization technique reduces the numerical diffusion added to the problem as the solution approaches the exact solution. Both streamline diffusion and crosswind diffusion are available. Streamline diffusion adds numerical diffusion along the direction of the flow velocity (that is, the diffusion is parallel to the streamlines). Crosswind diffusion adds diffusion in the direction orthogonal to the velocity.

Generally it is best to use consistent stabilization where possible. If convergence problems are still encountered, inconsistent stabilization can be used with a parametric or time-dependent solver that slowly eliminates this term.

	• Selection Information and Numerical Stabilization in the *COMSOL Multiphysics Reference Manual* • Other Dimensionless Numbers

TABLE 2-2: IMPORTANT DIMENSIONLESS NUMBERS RELATED TO THE STABILITY OF VARIOUS MICROFLUIDIC PROBLEMS.

DIMENSIONLESS NUMBER	SYMBOL	GLOBAL DEFINITION	CELL DEFINITION	NOTES
Reynolds number	Re	$\mathrm{Re} = \frac{\rho v L}{\mu}$	$\mathrm{Re}^c = \frac{\rho v h}{2\mu}$ `spf.cellRe`	Ratio of inertial forces to viscous forces. Laminar flow applies: $\mathrm{Re} < 10^3$ Creeping flow applies: $\mathrm{Re} \ll 1$ Stabilization required: $\mathrm{Re}^c > 1$
Peclet number (Heat Flow)	Pe	$\mathrm{Pe} = \frac{\rho c_p v L}{\kappa}$	$\mathrm{Pe}^c = \frac{\rho c_p v h}{2\kappa}$ `spf.cellPe`	Ratio of heat convection to thermal diffusivity, $\alpha = \kappa/(\rho c_p)$. Stabilization required: $\mathrm{Pe}^c > 1$
Peclet number (Mass Transport)	Pe	$\mathrm{Pe} = \frac{vL}{D}$	$\mathrm{Pe}^c = \frac{vh}{2D}$	Ratio of concentration convection to diffusion. Stabilization required: $\mathrm{Pe}^c > 1$

Symbol definitions: v is the characteristic velocity or cell velocity, r is the fluid density, L is the characteristic length scale for the problem, μ is the fluid viscosity, h is the element size, c_p is the heat capacity at constant pressure, κ is the thermal conductivity, and D is the diffusion constant. For anisotropic diffusion or conductivity an appropriate average is computed. The variables names assume the default name spf.

Other Dimensionless Numbers

A number of other dimensionless numbers are useful for describing fluid flows on the microscale. These numbers are summarized in Table 2-3.

TABLE 2-3: DIMENSIONLESS NUMBERS USEFUL FOR CHARACTERIZING MICROFLUIDIC FLOWS.

DIMENSION LESS NUMBER	SYMBOL	DEFINITION	NOTES
Bond number/ Eötvös number	Bo Eo	$\left.\begin{matrix}\mathrm{Bo}\\ \mathrm{Eo}\end{matrix}\right\} = \frac{\rho g L^2}{\sigma}$	Ratio of surface tension forces to body forces (usually gravity) for two-phase flow. Density can refer to density difference when considering buoyancy. At high Bond numbers surface tension has a minimal effect on the flow, ($\mathrm{Bo} \gg 1$), at low Bond numbers, surface tension dominates ($\mathrm{Bo} < 1$).
Capillary number	Ca	$\mathrm{Ca} = \frac{\mu v}{\sigma}$	Ratio of viscous forces to surface tension for two phase flow. At low capillary numbers ($\mathrm{Ca} < 10^{-5}$) flow in porous media is dominated by surface tension.
Dukhin number	Du	$\mathrm{Du} = \frac{K^{\sigma}}{K^{B}}$	Ratio of the surface conductivity contribution to the fluid bulk electric conductivity contribution in electrokinetic phenomena. For low Dukhin numbers ($\mathrm{Du} \ll 1$), surface conductivities can be neglected when modeling electrokinetic flows.
Knudsen number	Kn	$\mathrm{Kn} = \frac{\lambda}{L}$	Ratio of the gas mean free path to the characteristic length scale. Continuum flow occurs when Kn<0.01, slip flow occurs in the range 0.01<Kn<0.1, transitional flow occurs in the range 0.1<Kn<10 and Free Molecular Flow occurs when Kn>10. For more details see Modeling Rarefied Gas Flows.
Mach number	Ma	$\mathrm{Ma} = \frac{v}{a}$	Ratio of the convective speed to the speed of sound in the medium. The Laminar Flow interface in the Microfluidics Module can handle compressible flows with $\mathrm{Ma} < 0{,}3$. For higher Mach number flows the CFD Module is required.

Symbol definitions: ρ is the fluid density, g is the body force acceleration (usually the acceleration due to gravity), L is the characteristic length scale for the problem, σ is the surface tension coefficient, μ is the fluid viscosity, v is the characteristic velocity, K^{σ} is the surface conductivity, K^{B} is the bulk conductivity, λ is the mean free path, α is the thermal diffusivity ($\alpha=\kappa/(\rho c_p)$), c_p is the heat capacity at constant pressure, κ is the thermal conductivity, and T is the absolute temperature (ΔT is the characteristic temperature difference).

TABLE 2-3: DIMENSIONLESS NUMBERS USEFUL FOR CHARACTERIZING MICROFLUIDIC FLOWS.

DIMENSION LESS NUMBER	SYMBOL	DEFINITION	NOTES
Marangoni number	Mg	$\mathrm{Mg} = \frac{d\sigma L \Delta T}{dT\ \mu\alpha}$	Ratio of thermal surface tension forces to viscous forces. In the low Marangoni number range ($\mathrm{Mg} \ll 1000$) viscous forces dominate over surface tension gradients.
Ohnesorge /Laplace /Surataman numbers	Oh La Su	$\mathrm{Oh} = \frac{\mu}{\sqrt{\rho\sigma L}}$ $\left.\begin{matrix}\mathrm{La}\\ \mathrm{Su}\end{matrix}\right\} = \frac{1}{\mathrm{Oh}^2}$	Relates the inertial and surface tension forces to the viscous forces. Used to describe the breakup of liquid jets and sheets: at low Ohnesorge and Reynolds numbers the Rayleigh instability occurs, at high Ohnesorge and Reynolds numbers atomization occurs.
Weber number	We	$\mathrm{We} = \frac{\rho v^2 L}{\sigma}$	Ratio of inertial forces to surface tension forces. For small Weber numbers ($\mathrm{We} \ll 1$) surface tension dominates the flow.

Symbol definitions: ρ is the fluid density, g is the body force acceleration (usually the acceleration due to gravity), L is the characteristic length scale for the problem, σ is the surface tension coefficient, μ is the fluid viscosity, v is the characteristic velocity, K^{σ} is the surface conductivity, K^{B} is the bulk conductivity, λ is the mean free path, α is the thermal diffusivity ($\alpha=\kappa/(\rho c_p)$), c_p is the heat capacity at constant pressure, κ is the thermal conductivity, and T is the absolute temperature (ΔT is the characteristic temperature difference).

Modeling Microfluidic Fluid Flows

This section describes the modeling of fluid flows with the Navier Stokes or Stokes equations (the section Modeling Rarefied Gas Flows gives details on how to model rarefied flows). The following topics are covered:

- Selecting the Right Physics Interface
- Single-Phase Flow
- Multiphase Flow
- Porous Media Flow
- The Relationship Between the Physics Interfaces

	• Building a COMSOL Multiphysics Model in the *COMSOL Multiphysics Reference Manual* • Modeling Rarefied Gas Flows

Selecting the Right Physics Interface

COMSOL Multiphysics has a range of physics interfaces to use for fluid flow in a variety of circumstances. Often the selection of a particular physics interface implies certain assumptions about the equations of flow. If it is known in advance which assumptions are valid, then the appropriate physics interface can be added. However, when the flow type is unclear from the outset, or if it is difficult to reach a solution easily, starting with a simplified model and adding complexity subsequently is often a good approach. Using this approach the results of a simulation are tested against the underlying assumptions and against experimental results and the simulation can then be refined if necessary. For complex models it is often beneficial to take this approach even when the fluid flow is well characterized from the outset because a model with simplifying assumptions can be easier to solve initially. The solution process can then be fine-tuned for the more complex problem. Typically The Laminar Flow Interface is a good starting point for many problems.

The following sections describe the options available for simulating Single-Phase Flow, Multiphase Flow, and Porous Media Flow.

Single-Phase Flow

The **Fluid Flow** > **Single-Phase Flow** branch ( ) when adding a physics interface includes the Laminar and Creeping Flow interfaces.

The Laminar Flow Interface ( ) is used primarily to model slow-moving flow in environments without sudden changes in geometry, material distribution, or temperature. The Navier-Stokes equations are solved without a turbulence model. Laminar flow typically occurs at Reynolds numbers less than 1000. By default the flow is incompressible (see Figure 2-1).

The Creeping Flow Interface ( ) uses the same equations as the Laminar Flow interface with the additional assumption that the contribution of the inertia term is negligible. This is often referred to as Stokes flow and is appropriate for use when viscous flow is dominant, which is often the case in microfluidics applications. Creeping flow applies when the Reynolds number is much less than one. A creeping flow problem is significantly simpler to solve than a laminar flow problem — so it is best to make this assumption explicitly if it applies. By default the flow is incompressible (see below).

	By selecting the **Neglect Inertial Form (Stokes Flow)** checkbox, in the **Settings** window for **Laminar Flow** quickly convert a Laminar Flow interface into a Creeping Flow interface.

For both physics interfaces several additional options are available.

SHALLOW CHANNEL APPROXIMATION

Often you might want to simplify long, narrow channels by modeling them in 2D. The Use Shallow Channel Approximation option is useful as it includes a drag term to approximate the added affects given by thinness of the gap between one set of boundaries in comparison to the others.

COMPRESSIBLE FLOW

For compressible flow it is important that the density and any mass balances are well defined throughout the domain. Choosing to model incompressible flow simplifies the equations to be solved and decreases solution times. Most gas flows should be modeled as compressible flows; however, liquid flows can usually be treated as incompressible.

INCLUDE GRAVITY

Gravity can be included when required. It can be neglected in models dominated by other effects.

NON-NEWTONIAN FLOW

The physics interfaces also allow for easy definition of non-Newtonian fluid flow through access to the dynamic viscosity in the Navier–Stokes equations. The fluid can be modeled using the Power law, Carreau, Bingham–Papanastasiou, Herschel–Bulkley–Papanastasiou, and Casson–Papanastasiou models or by means of any expression that describes the dynamic viscosity appropriately. To use other non-Newtonian models or model viscoelastic flow, the Polymer Flow Module is recommended in addition to the Microfluidics Module. The different non-Newtonian models can be defined directly in the physics, or using the corresponding Material Model nodes.

Both physics interfaces also include a feature to compute a laminar velocity profile at arbitrarily shaped inlets and outlets, which makes models much easier to set up.

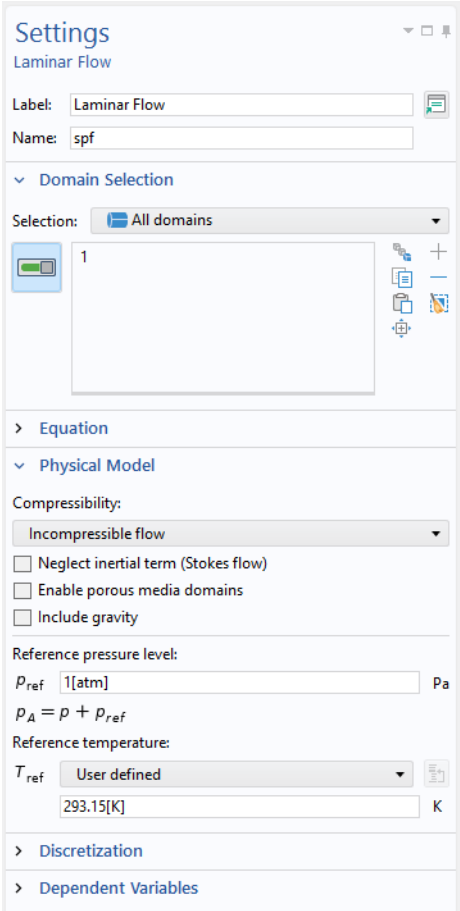


Figure 2-1: The Settings window for Laminar Flow. Model incompressible or compressible (Ma< 0.3) flow, and Stokes flow. Combinations are also possible.

Multiphase Flow

The **Multiphase Flow** branch ( ) enables the modeling of multiphase flows. These physics interfaces are included:

- The Laminar Two-Phase Flow, Level Set Interface ( ) (available under the **Two-Phase Flow, Level Set** branch ( )).
- The Laminar Two-Phase Flow, Phase Field Interface ( ) (available under the **Two-Phase Flow, Phase Field** branch ( )).

- The Laminar Three-Phase Flow, Phase Field Interface ( ) (available under the **Three-Phase Flow, Phase Field** branch( ))
- The Laminar Two-Phase Flow, Moving Mesh Interface ( ) (available under the **Two-Phase Flow, Moving Mesh** branch ( )).

The Two-Phase Flow interfaces can add surface tension forces (including the Marangoni effect) at the two fluid interface(s). A library of surface tension coefficients between some common substances is available.

For problems involving topological changes (for example, jet breakup), use either the Level Set or Phase Field interfaces. These techniques use an auxiliary function (the level set and phase field functions, respectively) to track the location of the interface, which is necessarily diffuse. The Level Set interface does not include surface tension force per default, and is recommended for use in larger scale problems with larger velocities, or when the effects of the gradient of the surface tension coefficient are relevant. The interface also includes a domain feature for porous domains. The phase field method is physically motivated and is usually more numerically stable than the level set method. It is can also be extended to more phases and is compatible with fluid-structure interactions.

The moving mesh method represents the interface as a boundary condition along a line or surface in the geometry. Because the physical thickness of phase boundaries is usually very small, for most practical meshes The Laminar Two-Phase Flow, Moving Mesh Interface describes the two-phase boundary the most accurately. However, it cannot accommodate topological changes in the boundary.

For all the Two and Three-Phase Flow interfaces, compressible flow is possible to model at speeds of less than 0.3 Mach. You can also choose to model incompressible flow by simplifying the equations to be solved. Stokes' law is also an option.

In each physics interface, the density and viscosity are specified for both fluids. You can easily use non-Newtonian models for any of the fluids, based on the Power law, Carreau, Bingham-Papanastasiou, Herschel-Bulkley-Papanastasiou, and Casson-Papanastasiou models, or using an arbitrary user-defined expression.

It is often advantageous to use more than one of these techniques to solve a problem — for example, a level set model for jet breakup could be checked prior to breakup by

a moving mesh model to ensure that the surface tension is captured accurately by the diffuse interface.

	Under the **Mathematics>Moving Interface** branch ( ) when adding an interface, The Level Set Interface ( ), The Level Set in Porous Media Interface ( ), The Phase Field in Fluids Interface ( ), and The Ternary Phase Field Interface ( ) are available in a form uncoupled with the equations of flow. These interfaces can be used to model phenomena in which other factors dominate over the fluid flow, such as some forms of phase separation.

Porous Media Flow

The **Porous Media and Subsurface Flow** branch ( ) has the physics interfaces to model flow in porous media. The flow can be modeled by Darcy's Law or the Brinkman Equations interfaces. Additionally the flow in a porous medium can be combined with laminar free flow in the Free and Porous Media Flow, Brinkman interface or the Free and Porous Media Flow, Darcy interface.

DARCY'S LAW

The Darcy's Law Interface ( ) is used to model fluid movement through interstices in a porous medium in the case where the fluid viscosity dominates over its inertia. Together with the continuity equation and the equation of state for the pore fluid (or gas) Darcy's law is used to model low velocity flows, for which the pressure gradient is the dominant driving force (typically when the Reynolds number of the flow is less than one). The penetration of reacting gases in a tight catalytic layer, such as a washcoat or membrane, is an example in which Darcy's law applies. Often Darcy's law is applicable for microfluidic applications, as it is appropriate for the limit of small pore size.

BRINKMAN EQUATIONS

The Brinkman Equations Interface ( ) is used in situations where the fluid inertia, or other effects such as body forces, can no longer be neglected. Fluid penetration of filters and packed beds are applications for this physics interface. The Brinkman equations are similar in form to the Navier Stokes equations. Figure 2-2 shows the **Settings** window for the Brinkman Equations interface.

For low Reynolds number flows in which other terms in the Brinkman equations are necessary the Neglect Inertial Term (Stokes–Brinkman Flow) feature can be selected to neglect the inertial term in the equations (this is selected by default). The flow is treated as incompressible by default, but compressible flow can be enabled by selecting **Compressible Flow (Ma<0.3)**. When using the compressible flow feature the fluid density must be defined as a function of the local pressure.

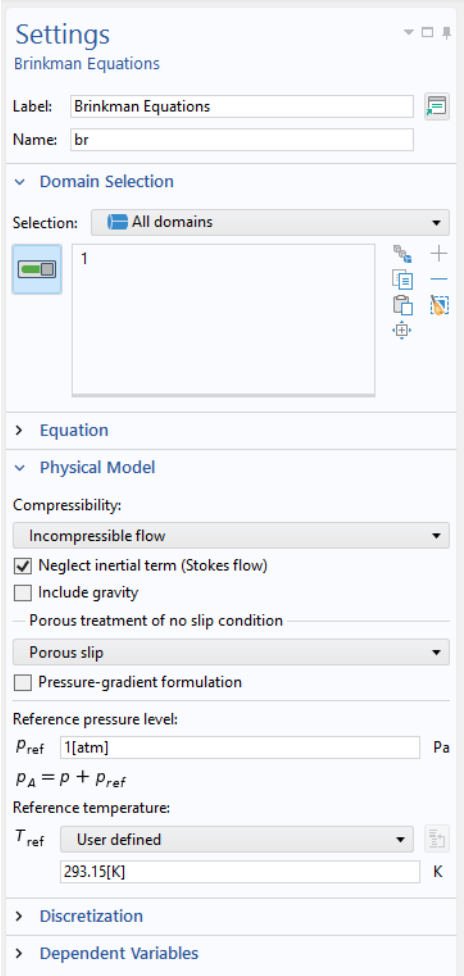


Figure 2-2: The Settings window for Brinkman Equations. Model incompressible or compressible (Ma<0.3) flow, and Stokes flow. Other combinations are also possible.

FREE AND POROUS MEDIA

The Free and Porous Media Flow, Brinkman Interface ( ) has predefined couplings between the Brinkman Equations interface and the Laminar Flow interface. Porous regions of the models are included by adding a Porous Medium node with the appropriate selections to the model. The default Fluid Properties node can then be used to define regions of free laminar flow. This physics interface has all the options from both The Laminar Flow Interface and The Brinkman Equations Interface. An example application area for this physics interface would be a catalytic converter.

It should be noted that if the porous medium is large in comparison to the free channel, and the results in the region of the interface are not of interest, then it is possible to couple a Laminar Flow interface to the Darcy's Law interface using The Free and Porous Media Flow, Darcy Interface ( ). This makes the model computationally cheaper.

The Relationship Between the Physics Interfaces

Several of the physics interfaces vary only by one or two default settings (see Table 2-4 and Table 2-5) in the **Physical Model** section, which are selected either from a checkbox or list. For the Single-Phase Flow branch, the Laminar Flow and Creeping Flow interfaces have the same *Name* (`spf`), and this is the same for two of the Two-Phase Flow interfaces. In the Porous Media Flow branch the Free and Porous Media Flow, Brinkman interface combines a Laminar Flow interface with a Brinkman Equations interface (see Table 2-6), and the Free and Porous Media Flow, Darcy interface combines a Laminar Flow interface with Darcy's Law interface.

TABLE 2-4: THE SINGLE-PHASE FLOW PHYSICAL MODEL DEFAULT SETTINGS.

PHYSICS INTERFACE LABEL	NAME	COMPRESSIBILITY	NEGLECT INERTIAL TERM (STOKES FLOW)
Laminar Flow	spf	Compressible flow (Ma<0.3)	None
Creeping Flow	spf	Compressible flow (Ma<0.3)	Stokes Flow

TABLE 2-5: TWO-PHASE FLOW PHYSICAL MODEL DEFAULT SETTINGS.

PHYSICS INTERFACE LABEL	NAME	MULTIPHASE FLOW MODEL	COMPRESSIBILITY	NEGLECT INERTIAL TERM (STOKES FLOW)
Laminar, Two-Phase Flow, Level Set	tpf	Two phase flow, level set	Incompressible flow	None
Laminar, Two-Phase Flow, Phase Field	tpf	Two phase flow, phase field	Incompressible flow	None
Laminar, Three-Phase Flow, Phase Field	tfpf	Three phase flow, phase field	Incompressible flow	None
Laminar, Two-Phase Flow, Moving Mesh	spf	not applicable	Incompressible flow	None

TABLE 2-6: THE POROUS MEDIA FLOW DEFAULT SETTINGS.

PHYSICS INTERFACE LABEL	NAME	COMPRESSIBILITY	NEGLECT INERTIAL TERM	PORE SIZE
Darcy's Law	dl	n/a	n/a	Low porosity and low permeability, slow flow
Brinkman Equations	br	Incompressible flow	Yes — Stokes–Brinkman	High permeability and porosity, faster flow
Free and Porous Media Flow, Brinkman	fp	Incompressible flow	Not selected	High permeability and porosity, fast flow
Free and Porous Media Flow, Darcy	nsd	Incompressible/ Compressible	Not selected	Low porosity and low permeability, slow flow

Modeling Coupled Phenomena in Microfluidics

In this section:

- Chemical Transport and Reactions
- Electrohydrodynamics
- Heat Transfer
- Coupling to Other Physics Interfaces

	See The AC/DC Interfaces in the *COMSOL Multiphysics Reference Manual* for details, including theory, about The Electrostatics Interface and The Magnetic Fields Interface, which are included with the basic COMSOL Multiphysics license and discussed in this section.

Chemical Transport and Reactions

In the Microfluidics Module, The Transport of Diluted Species Interface ( ) and The Transport of Diluted Species in Porous Media Interface ( ) are available for modeling the transport of chemical species and ions. The assumption in these physics interfaces is that one component, a solvent, is present in excess (typically more than 90 mol%). This means that the mixture properties, such as density and viscosity, are independent of concentration. To model concentrated species, the Chemical Reaction Engineering Module is recommended in addition to the Microfluidics Module.

By default the Transport of Diluted Species interface accounts for the diffusion of species by Fick's law and convection due to bulk fluid flow (see Figure 2-3). The fluid velocity field can be coupled from another physics interface (for example, Laminar Flow) by means of a domain level model input. The migration of ionic species in an electric field can also be added by selecting the appropriate checkbox in the Settings window for the physics interface — in this case an additional Electrostatics interface is usually coupled into the problem by an additional model input.

Chemical reactions can be added to the physics interface at the domain level by the Reactions node, which requires the Chemical Reaction Engineering Module. This allows you to specify expressions for the consumption or production of species in terms

of their concentration, the concentration of other species, and other model parameters, such as the temperature.

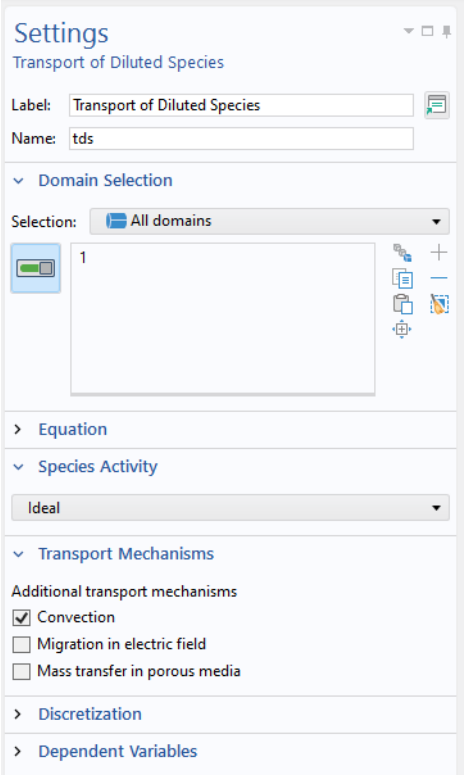


Figure 2-3: The Settings window for Transport of Diluted Species, with Convection selected as the Transport Mechanism by default.

STABILIZATION SETTINGS FOR DILUTED SPECIES TRANSPORT

For some laminar flow problems it can be useful to change the settings for the dilute species transport stabilization. To do this, click the **Show More Options** button (👁) and select **Stabilization** in the **Show More Options** dialog. A **Consistent stabilization** section is now visible in the Transport of Diluted species settings, and in some cases it can be desirable to change the settings for the crosswind diffusion. By default the **Crosswind diffusion type** is set to **Do Carmo and Galeão**. This type of crosswind diffusion reduces undershoot and overshoot to a minimum but can in rare cases give equations systems that are difficult to fully converge. The alternative option, **Codina** is less diffusive and so should be used if the species transport is highly convective, or if

convergence problems occur. This option can result in more undershoot and overshoot and is also less effective for anisotropic meshes.

For both consistent stabilization methods, the **Equation residual** can also be changed. **Approximate residual** is the default setting and it means that derivatives of the diffusion tensor components are neglected. This setting is usually accurate enough and is faster to compute. If required, select **Full residual** instead.

Electrohydrodynamics

Electrohydrodynamics is a general term describing phenomena that involve the interaction between solid surfaces, ionic solutions, and applied electric and magnetic fields. Electrohydrodynamics is frequently employed in microfluidic devices to manipulate fluids and move particles for sample handling and chemical separation.

Electrokinetics refers to a range of fluid flow phenomena involving electric fields. These include electroosmosis, electrothermal effects, electrophoresis, and dielectrophoresis. *Electroosmosis* describes the motion of fluids induced by the forces on the charged EDLs at the surfaces of the fluid. *Electrothermal effects* occur in a conductive fluid where the temperature is modified by Joule heating from an AC electric field. This creates variations in conductivity and permittivity and thus Coulomb and dielectric body forces. *Electrophoresis* and *dielectrophoresis* describe the motion of charged and polarized particles in a nonuniform AC or DC applied field.

Magnetohydrodynamics refers to fluid flow phenomena involving magnetic fields. *Magnetophoresis* is the motion of diamagnetic particles in a nonuniform magnetic field and is commonly used for magnetic bead separation.

Table 2-7 summarizes these categories. Although these examples describe specific multiphysics couplings, COMSOL Multiphysics is not limited to these cases — for example, it is possible to include both magnetic and electric fields to simulate electromagnetophoresis.

TABLE 2-7: ELECTROHYDRODYNAMIC PHENOMENA.

TYPE OF FIELD/FORCE	DC	AC
ELECTRIC FIELD (ELECTROKINETICS)		
Surface force on fluid	Electroosmosis	AC electroosmosis
Force on suspended particles	Electrophoresis / Dielectrophoresis	AC Electrophoresis /AC Dielectrophoresis
Body force on fluid	-	Electrothermal

TABLE 2-7: ELECTROHYDRODYNAMIC PHENOMENA.

TYPE OF FIELD/FORCE	DC	AC
Magnetic Field		
Force on suspended particles	Magnetophoresis	-

See The AC/DC Interfaces in the *COMSOL Multiphysics Reference Manual* for details, including theory, about The Electrostatics Interface and The Magnetic Fields Interface, which are included with the basic COMSOL license and discussed in this section.

ELECTROOSMOSIS

When a polar liquid (such as water) and a solid surface (such as glass or a polymer-based substrate) come into contact, charge transfer occurs between the surface and the electrolytic solution. At finite temperature the charges on the surface are not screened perfectly by the ions in the liquid and a finite thickness *electric double layer (EDL)* or *Debye layer* develops. *Electroosmosis* is the process by which motion is induced in a liquid due to the body force acting on the EDL in an electric field.

A complete model of the system includes the space charge layer explicitly. The electric potential is the solution of a nonlinear partial differential equation, the Poisson–Boltzmann equation, which can be solved by coupling an Electrostatics interface to a Transport of Diluted Species interface (with migration enabled) for the ion species. The software then computes the forces on the fluid and a further coupled Laminar Flow or Creeping Flow interface is used to compute the overall fluid flow. In practice this approach is only possible for nanoscale channels — as typically the EDL thickness is 1–10 nm.

The Poisson–Boltzmann equation is sometimes linearized — this is referred to as the Debye–Hückel approximation which applies when $ze\zeta \ll k_B T$, where ζ is the potential at the surface of the moving volume of fluid (the *zeta potential*). At room temperature this corresponds to the limit $\zeta \ll 26$ mV. Note that there is a layer of immobile ions trapped adjacent to the surface (the *Stern layer*, which is of order one hydrated ion radius thick) with an associated volume of immobile fluid; this means that ζ is not simply the wall potential. ζ is usually determined experimentally from electroosmotic flow measurements.

The Poisson–Boltzmann equation has a characteristic length scale — the Debye length, λ_D:

$$\lambda_D = \sqrt{\frac{\varepsilon k_B T}{2z^2 e^2 c_\infty}}$$

where k_B is Boltzmann's constant, T is the temperature, z is the ion's valence number, e is the electron charge, and c_∞ is the ion's molar concentration in the bulk solution. When the Debye length is small compared to the channel thickness, the electroosmotic flow velocity can be modeled by the *Helmholtz–Smoluchowski equation*:

$$u_{eo} = \frac{\varepsilon\zeta}{\mu}E$$

where E is the applied electric field and μ is the liquid's dynamic viscosity. From this equation, the electroosmotic mobility is naturally defined as:

$$\mu_{eo} = \frac{\varepsilon\zeta}{\mu} \tag{2-1}$$

The Laminar Flow and Creeping Flow interfaces include a wall boundary condition option for an Electroosmotic Velocity boundary condition. This enables you to specify the external electric field (which can be manually specified or coupled from an Electrostatics interface) and the electroosmotic mobility to define an electroosmotic flow.

Further details of the theory of electroosmosis can be found in Ref. 1 and Ref. 2.

AC ELECTROOSMOSIS

Because an alternating electric field does not generate a net force on the EDL, AC electroosmosis is not used for fluid transport in microfluidics. However, the back-and-forth movements an AC field generates are useful for mixing purposes. To model AC electroosmotic flow when the frequency of the electric field is sufficiently low, the same approaches can be taken as for DC electroosmosis. An Electrostatics interface should still be used to calculate the electric field, but when this is coupled into other physics interfaces, the AC dependence should be explicitly added using an expression. With increasing frequency, AC electroosmosis becomes less important so this approach is valid for most practical examples.

	Electroosmotic Micromixer: Application Library path **Microfluidics_Module/Micromixers/electroosmotic_mixer**

ELECTROPHORESIS

Electrophoresis describes the motion of charged particles or molecules suspended in a liquid due to an applied electric field.

In COMSOL Multiphysics it is easy to calculate the electrophoretic velocity for spherical particles for the cases when the Debye length is much smaller or much larger than the particle size. If the surface conductivity of the particle can be neglected (this is sometimes referred to as the limit or small Dukhin number) the electrophoretic velocity (the particle velocity relative to the bulk flow) is given by:

$$\mathbf{u}_{\mathrm{ep}} = \frac{2}{3}\mu_{\mathrm{eo}} f\left(\frac{a}{\lambda_D}\right)\mathbf{E}$$

where a is the radius of the particle, $\mathbf{E}$ is the electric field, and $f(a/\lambda_{\mathrm{D}})$ is known as Henry's function (note that $f(a/\lambda_D)$ is often written as $f(\kappa a)$ where $\kappa = 1/\lambda_D$). Henry's function takes the value of 1 in the limiting case where $a \ll \lambda_D$ (often known as the Hückel approximation) and $3/2$ in the case where $a \gg \lambda_D$ (this is equivalent to Equation 2-1 and is referred to as the Smoluchowski approximation). Note that if λ_D is large compared to the fluid volume, the charge is effectively unscreened and the electric force is simply that due to the charge on the molecule. The following result is obtained from the force balance between the Stokes drag and the electric force for an unscreened charged particle:

$$\mathbf{u}_{\mathrm{ep}} = \frac{q}{6\pi\mu a}\mathbf{E}$$

where q is the charge on the molecule and μ is the fluid viscosity. Further details of the theory of electroosmosis can be found in Ref. 2.

These velocity fields can be computed directly from an electric field calculated by the Electrostatics interface. If necessary the velocity can be added to the flow velocity field to compute the net particle velocity.

DIELECTROPHORESIS

Dielectrophoresis (DEP) describes the motion of polarizable particles suspended in a fluid with an applied nonuniform electric field. The electric field induces a dipole moment on the particles, which in turn produces a net force. In the following

discussion the general case of AC electrophoresis is treated, which is more commonly used for practical reasons (see Ref. 1 for further details).

For a DC field these results can be applied if $\mathbf{E}_{\text{rms}}=\mathbf{E}$ is used.

The time-dependent dielectrophoretic force acting on a particle in an applied field is given by (Ref. 1):

$$\mathbf{F}_{\text{DEP}}(t) = 2\pi\varepsilon_m a^3 K(\varepsilon_m,\varepsilon_p)\nabla(\mathbf{E}(t)\cdot\mathbf{E}(t)) \tag{2-2}$$

where ε_m and ε_p are the complex permittivities of the medium and the particle, respectively; a is the radius of the particle's equivalent homogeneous sphere; and $K(\varepsilon_m,\varepsilon_p)$ is the Clausius–Mossotti function. The complex permittivity, ε^*, for an isotropic homogeneous dielectric is

$$\varepsilon^* = \varepsilon - i\frac{\sigma}{\omega}$$

where ε is the electric permittivity, σ is the electric conductivity, and ω is the angular field frequency. The Clausius–Mossotti function is given by:

$$K(\varepsilon_m,\varepsilon_p) = \frac{\varepsilon_p-\varepsilon_m}{\varepsilon_p+2\varepsilon_m}$$

which depends on the particle's complex permittivity, ε_p, and that of the medium, ε_m.

Taking the time average of Equation 2-2 gives the time-averaged force:

$$\langle\mathbf{F}_{\text{DEP}}(t)\rangle = 2\pi\varepsilon_m r_0 \text{Re}(K(\varepsilon_m,\varepsilon_p))\nabla(\mathbf{E}_{\text{rms}}\cdot\mathbf{E}_{\text{rms}})$$

By balancing this force with the Stokes drag force the dielectrophoretic velocity is obtained:

$$\mathbf{u}_{\text{DEP}} = \frac{\varepsilon_m r_0 \text{Re}(K(\varepsilon_m,\varepsilon_p))\nabla(\mathbf{E}_{\text{rms}}\cdot\mathbf{E}_{\text{rms}})}{3\mu}$$

where μ is the dynamic viscosity.

The value of $\mathbf{E}_{\text{rms}}$ can be computed from an Electrostatics interface in which the root mean square (RMS) voltages are applied as boundary conditions. The gradient of the field can then be computed term by term from the spatial derivatives of an expression

for the dot product of the electric field with itself. Finally the dielectrophoretic velocity term can be added to the velocity field to compute the particle velocity field.

MAGNETOPHORESIS

Particles with an induced or permanent magnetization can be moved relative to a fluid flow by the application of an external, inhomogeneous magnetic field. This process is analogous to dielectrophoresis and is usually termed magnetophoresis. In the case of a nonconducting particle, in a static, irrotational external applied field, $\mathbf{H}_{\text{ext}}$, the magnetophoretic force is given by (Ref. 1):

$$\mathbf{F}_{MAP} = 2\pi\mu_m K(\mu_m, \mu_p) a^3 \nabla(\mathbf{H}_{\text{ext}} \cdot \mathbf{H}_{\text{ext}})$$

where μ_m and μ_p are the permeabilities of the medium and the particle, respectively (usually $\mu_m = \mu_0$); a is the radius of the particle's equivalent homogeneous sphere; and $K(\mu_m,\mu_p)$ is the Clausius–Mossotti function. Note that the external magnetic field, $\mathbf{H}_{\text{ext}}$, should be distinguished from the local field $\mathbf{H}$ which includes contributions from the particle itself. In this case the Clausius–Mossotti function is given by:

$$K(\mu_m, \mu_p) = \frac{\mu_p - \mu_m}{\mu_p + 2\mu_m}$$

By balancing this force with the Stokes drag force the magnetophoretic velocity is obtained:

$$\mathbf{u}_{MAP} = \frac{\mu_m r_0 K(\mu_m, \mu_p) \nabla(\mathbf{H}_{ext} \cdot \mathbf{H}_{ext})}{3\mu}$$

where μ is the dynamic viscosity.

The value of $\mathbf{H}_{\text{ext}}$ can be computed from a Magnetic Fields or a Magnetic Fields, No Currents interface.

	The Magnetic Fields, No Currents interface requires the AC/DC Module.

	The Magnetic Fields Interface in the *COMSOL Multiphysics Reference Manual*

The gradient of the field can then be computed term by term from the spatial derivatives of an expression for the dot product of the magnetic field with itself. Finally the magnetophoretic velocity term can be added to the velocity field to compute the particle velocity field.

ELECTROTHERMALLY-DRIVEN FLOW

Electrothermal body forces arise from electrically generated, nonuniform Joule heating, which creates variations in conductivity and permittivity and thus Coulomb and dielectric body forces. It is possible to determine the resulting fluid motion by solving the Navier–Stokes equations with an additional electrothermal body force term. The electric field is once again assumed to be quasistatic and can be coupled in from an Electrostatics interface.

The electrothermal force is given by:

$$\mathbf{F} = -\frac{1}{2}\left[\left(\frac{\nabla\sigma}{\sigma} + \frac{\nabla\varepsilon}{\varepsilon}\right)\cdot\mathbf{E}\frac{\varepsilon\mathbf{E}}{1+(\omega\tau)^2} + \frac{1}{2}|\mathbf{E}|^2\nabla\varepsilon\right]$$

where σ is the conductivity, ε is the fluid's permittivity, ω is the angular frequency of the electric field, and $\tau = \varepsilon/\sigma$ is the fluid's charge-relaxation time. The electric-field vector $\mathbf{E}$ contains the amplitude and direction of the AC electric field but not its instantaneous value.

Because of the heating, ε and σ are temperature dependent, and their gradients are functions of the temperature gradient: $\nabla\varepsilon = (\partial\varepsilon/\partial T)\nabla T$ and $\nabla\sigma = (\partial\sigma/\partial T)\nabla T$. With water, for example, the relative change rates for the permittivity and the conductivity are $(1/\varepsilon)(\partial\varepsilon/\partial T) = -0.004\ 1/\mathrm{K}$ and $(1/\sigma)(\partial\sigma/\partial T) = 0.02\ 1/\mathrm{K}$, respectively.

ELECTROWETTING

The contact angle of a two-fluid interface with a solid surface is determined by the balance of the forces at the contact point. The equilibrium contact angle, θ_0, is given by Young's equation:

$$\gamma_{s1} + \sigma_{12}\cos\theta_0 = \gamma_{s2}$$

Here γ_{s1} is the surface energy per unit area between fluid 1 and the solid surface, γ_{s2} is the surface energy per unit area between fluid 2 and the solid surface, and σ_{12} is the surface tension at the interface between the two fluids.

In *electrowetting* the balance of forces at the contact point is modified by the application of a voltage between a conducting fluid and the solid surface. For many

applications the solid surface consists of a thin dielectric deposited onto a conducting layer; this is often referred to as *electrowetting on dielectric* (EWOD). In this case, the capacitance of the dielectric layer dominates over the double layer capacitance at the solid-liquid interface (Ref. 3). The energy stored in the capacitor formed between the conducting liquid and the conducting layer in the solid reduces the effective surface energy of the liquid to which the voltage is applied. For the case when a voltage difference occurs between fluid 1 and the conductor beyond the dielectric Young's equation is modified as follows:

$$\gamma_{s1} - \frac{\varepsilon V^2}{2d_f} + \sigma_{12} \cos\theta_{\mathrm{ew}} = \gamma_{s2}$$

Here ε is the permittivity of the dielectric, V is the potential difference applied, and d_f is the dielectric thickness. This equation can be rewritten as

$$\cos\theta_{\mathrm{ew}} = \cos\theta_0 + \frac{\varepsilon V^2}{2\sigma_{12} d_f} \tag{2-3}$$

Electrowetting can therefore be used to modify the contact angle dynamically by changing the applied voltage.

The EWOD applications can be modeled by using Equation 2-3 as an expression for the contact angle. This can simply be entered as the value of the contact angle in the Two-Phase Flow interface that is being used. Note that the software automatically handles a time varying voltage in this expression.

For step-by-step instructions, see *Electrowetting Lens*: Application Library path **Microfluidics_Module/Two-Phase_Flow/electrowetting_lens**.

Heat Transfer

It is often necessary to consider the effect of heat flow and temperature-dependent material properties (such as the viscosity or the surface tension) in microfluidic systems. The COMSOL Multiphysics base package includes physics interfaces for heat transfer in incompressible fluids and solids. The Heat Transfer Module is required in addition to this module to model heat flow in compressible fluids and to include viscous heating terms. This section describes how to couple heat transfer to microfluidics models using the functionality available in the COMSOL Multiphysics base package and the Microfluidics Module.

The Heat Transfer interface includes the equations for heat transfer in both fluid and solid domains. To model a system consisting of both solid and liquid domains add a single Heat Transfer interface and then add nodes for Heat Transfer in Solids and Heat Transfer in Fluids with selections corresponding to the solid and fluid domains respectively. For a fluid domain the convective flow is coupled into domain by selecting the velocity field from a corresponding Laminar Flow or Creeping Flow interface.

The fluid domain models the heat transfer including both convection and conduction according to the equation:

$$\rho C_p\left(\frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla)T\right) = -(\nabla \cdot \mathbf{q}) + Q$$

where, ρ is the fluid density (SI unit: kg/m^3), C_p is the specific heat capacity at constant pressure (SI unit: J/(kg·K)), T is absolute temperature (SI unit: K), $\mathbf{u}$ is the velocity vector (SI unit: m/s), $\mathbf{q}$ is the heat flux by conduction (SI unit: W/m^2), and Q contains heat sources other than viscous heating (SI unit: W/m^3). For a solid domain the following equation applies:

$$\rho C_p \frac{\partial T}{\partial t} = -(\nabla \cdot \mathbf{q}) + Q$$

When using the heat transfer in solids and in fluids domain properties the software automatically includes the heat transfer between the solid and the fluid. It is important to include the correct thermal boundary conditions on regions where fluid flows into or out of a domain, typically a Temperature condition for an inlet and an Outflow condition for an outlet.

For a detailed discussion of the fundamentals of heat transfer, see Ref. 4. More details of the heat transfer capabilities can be found in The Heat Transfer Interfaces in the *COMSOL Multiphysics Reference Manual*.

Coupling to Other Physics Interfaces

The COMSOL Multiphysics software is not limited to the common couplings described in this chapter — there are many other phenomena that can be easily modeled in microfluidics. In many cases, physics interfaces can be coupled simply by entering expressions from one physics interface (such as the local temperature) into fields in another physics interface (for example in the **Model Inputs** section of a **Fluid Properties** node). Additionally, COMSOL Multiphysics includes powerful coupling

operators that enable physics interfaces to be linked by projections, extrusions, or scalar quantities such as integrals and global averages.

	Nonlocal Couplings and Coupling Operators in the *COMSOL Multiphysics Reference Manual*

Modeling Rarefied Gas Flows

In this section:

- The Flow Regimes
- Slip Flow
- References for the Theory of Microfluidics

The Flow Regimes

Rarefied gas flow occurs when the mean free path, λ, of the molecules becomes comparable with the length scale of the flow, l. There are four flow regimes depending on the value of the Knudsen number, $\mathrm{Kn} = \lambda/l$ (Ref. 5):

- Continuum flow ($\mathrm{Kn} < 0.01$)
- Slip flow ($0.01 < \mathrm{Kn} < 0.1$)
- Transitional flow ($0.1 < \mathrm{Kn} < 10$)
- Free molecular flow ($\mathrm{Kn} > 10$)

These flow regimes are shown in Figure 2-4. In the *continuum flow* regime the Navier–Stokes equations are applicable, as discussed in Modeling Microfluidic Fluid Flows. Gases flowing in the slip flow regime can be modeled using the Navier–Stokes equations with modified boundary conditions. The Slip Flow interface is included with the Microfluidics Module and can be used to model gas flows at these moderate Knudsen numbers. The Molecular Flow Module includes the Transitional Flow and the Free Molecular Flow interfaces, which can be used to model fully kinetic gas flows, at Knudsen numbers greater than 0.1.

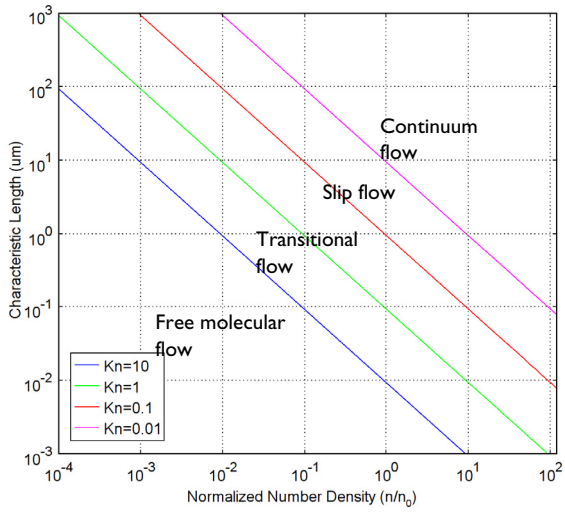


Figure 2-4: A plot showing the main fluid flow regimes for rarefied gas flows. Different regimes are separated by lines of constant Knudsen numbers. The number density of the gas is normalized to the number density of an ideal gas at a pressure of 1 atmosphere and a temperature of 0°C (n_0).

Slip Flow

In the slip flow regime, the Navier–Stokes equations can still be used with modified boundary conditions to account for rarefaction effects close to the wall. A layer of rarefied gas with a size similar to the mean free path develops close to the wall — this is termed the *Knudsen layer*. The Navier–Stokes equations are not applicable in this layer, but the flow outside the layer can be described by extrapolating the bulk gas flow toward the wall and applying Maxwell's slip boundary condition at the wall (Ref. 5). For thermal flows the von Smoluchowski temperature jump boundary condition must also be applied (Ref. 5).

To model flows in the slip flow regime use the Slip Flow interface. That physics interface can be used to model isothermal and nonisothermal flows with or without explicit modeling of thermal processes in adjacent solid domains. To model isothermal flows use the Temperature boundary condition on all external model surfaces, with the temperature set equal to the fluid temperature. The Slip Wall and External Slip Wall boundary conditions are used to model slip on interior and exterior model boundaries respectively. These boundary conditions include thermal creep or transpiration, viscous

slip, and the von Smoluchowski temperature jump. The slip coefficients can be specified directly or by means of Maxwell's model. For further details see The Slip Flow Interface and Theory for the Slip Flow Interface.

- The Temperature boundary condition is described for the Heat Transfer interface in the *COMSOL Multiphysics Reference Manual*.
- Slip Velocity

References for the Theory of Microfluidics

1. H. Bruus, *Theoretical Microfluidics*, Oxford University Press, 2008.

2. R.F. Probstein, *Physicochemical Hydrodynamics: An Introduction*, 2nd ed., Wiley-Interscience, 2003.

3. F. Mugele and J.C. Baret, "Electrowetting: from basics to applications", *J. Phys. Condens. Matter*, vol. 17, pp. R705–R774, 2005.

4. F.P. Incropera and D.P. DeWitt, *Fundamentals of Heat and Mass Transfer*, 4th ed., John Wiley & Sons, 1996.

5. G. Kariadakis, A. Beskok, and N. Aluru, *Microflows and Nanoflows*, Springer Science and Business Media, 2005.

3

Single-Phase Flow Interfaces

There are several Fluid Flow interfaces available with the Microfluidics Module. These are grouped by type and found under the **Fluid Flow** > **Single-Phase Flow** branch ( ) when adding a physics interface. See Modeling Microfluidic Fluid Flows to help you select which physics interface to use.

In this chapter:

- The Laminar Flow and Creeping Flow Interfaces
- The Potential Flow Interface
- Theory for the Single-Phase Flow Interfaces
- Theory for the Potential Flow Interface

The Laminar Flow and Creeping Flow Interfaces

In this section:

- The Creeping Flow Interface
- The Laminar Flow Interface
- Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow

- Theory for the Single-Phase Flow Interfaces

In the *COMSOL Multiphysics Reference Manual*, see Table 2-4 for links to common sections such as **Discretization**, **Consistent Stabilization**, **Inconsistent Stabilization**, and **Advanced Settings** sections, some of them accessed by clicking the **Show** button ( ) and choosing the applicable option. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

The Creeping Flow Interface

The **Creeping Flow (spf)** interface ( ) is used for simulating fluid flows at very low Reynolds numbers for which the inertial term in the Navier–Stokes equations can be neglected. Creeping flow, also referred to as Stokes flow, occurs in systems with high viscosity or small geometrical length scales (for example, in microfluidics and MEMS devices). The fluid can be compressible or incompressible, as well as Newtonian or non-Newtonian.

The equations solved by the Creeping Flow interface are the Stokes equations for conservation of momentum and the continuity equation for conservation of mass.

The Creeping Flow interface can be used for stationary and time-dependent analyses.

The main feature is the **Fluid Properties** node, which adds the Stokes equations and provides an interface for defining the fluid material and its properties. Except where noted below, see The Laminar Flow Interface for all other settings.

PHYSICAL MODEL

By default, the **Neglect inertial term (Stokes flow)** checkbox is selected. If unchecked, the inertial terms are included in the computations.

DISCRETIZATION

By default, the Creeping Flow interface uses **P2+P1** elements. Contrary to general laminar and turbulent single-phase flow simulations employing purely linear P1+P1 elements, P2+P1 elements are well suited for most creeping flow simulations but are not in general fully conservative. Full conservation properties and high accuracy is obtained by selecting P2+P2 or P3+P3 elements.

Note that P1+P1, P2+P2, and P3+P3 discretizations (the so-called equal order interpolations) require streamline diffusion to be active.

	• The Laminar Flow Interface • Theory for the Single-Phase Flow Interfaces

	• *Transport in an Electrokinetic Valve*: Application Library path **Microfluidics_Module/Fluid_Flow/electrokinetic_valve** • *Controlled Diffusion Separator*: Application Library path **Microfluidics_Module/Micromixers/controlled_diffusion_separator**

The Laminar Flow Interface

The **Laminar Flow (spf)** interface ( ) is used to compute the velocity and pressure fields for the flow of a single-phase fluid in the laminar flow regime. A flow remains laminar as long as the Reynolds number is below a certain critical value. At higher Reynolds numbers, disturbances have a tendency to grow and cause transition to turbulence. This critical Reynolds number depends on the model, but a classical example is pipe flow, where the critical Reynolds number is known to be approximately 2000.

The physics interface supports incompressible flow, weakly compressible flow (the density depends on temperature but not on pressure), and compressible flow at low Mach numbers (typically less than 0.3). It also supports flow of non-Newtonian fluids.

The equations solved by the Laminar Flow interface are the Navier–Stokes equations for conservation of momentum and the continuity equation for conservation of mass.

The Laminar Flow interface can be used for stationary and time-dependent analyses. Time-dependent studies should be used in the high-Reynolds number regime as these flows tend to become inherently unsteady.

When the Laminar Flow interface is added, the following default nodes are also added in the **Model Builder**: **Fluid Properties**, **Wall** (the default boundary condition is **No slip**), and **Initial Values**. Other nodes that implement, for example, boundary conditions and volume forces, can be added from the **Physics** toolbar or from the context menu displayed when right-clicking **Laminar Flow**.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Physics interface variables can be referred to using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `spf`.

About the Physics Interface Label Names

The label for a single-phase flow interface (the node name in the Model Builder) is dynamic and is reset according to the turbulence model and the neglect inertial term (Stokes flow) property set at the physics interface level. The availability also depends on the software license.

If the **Neglect inertial term (Stokes flow)** checkbox is selected, then the Label changes to **Creeping Flow**, which is the same Label that displays when that interface is added from the Model Wizard or Add Physics window.

PHYSICAL MODEL

Compressibility

Depending of the fluid properties and the flow regime, three options are available for the **Compressibility** option. In general the computational complexity increases from **Incompressible flow** to **Weakly compressible flow** to **Compressible flow (Ma<0.3)** but the underlying hypotheses are increasingly more restrictive in the opposite direction.

When the **Incompressible flow** option (default) is selected, the incompressible form of the Navier–Stokes and continuity equations is applied. In addition, the fluid density is

evaluated at the **Reference pressure level** defined in this section. The **Reference temperature** is set to 293.15 K.

The **Weakly compressible flow** option models compressible flow when the pressure dependency of the density can be neglected. When selected, the compressible form of the Navier–Stokes and continuity equations is applied. In addition, the fluid density is evaluated at the **Reference pressure level** defined in this section.

When the **Compressible flow (Ma<0.3)** option is selected, the compressible form of the Navier–Stokes and continuity equations is applied. $\mathrm{Ma} < 0.3$ indicates that the inlet and outlet conditions, as well as the stabilization, may not be suitable for transonic and supersonic flow. For more information, see The Mach Number Limit.

Neglect Inertial Term (Stokes Flow)

For low Reynolds number flows, the inertial terms in the Navier–Stokes equations may be neglected.

Porous Media Domains

With the addition of various modules, the **Enable porous media domains** checkbox is available. Selecting this option, a **Fluid and Matrix Properties** node, a **Mass Source** node, and a **Forchheimer Drag** subnode are added to the physics interface. These are described for the **Brinkman Equations** interface in the respective module's documentation. The **Fluid and Matrix Properties** can be applied on all domains or on a subset of the domains.

Porous Treatment of No Slip Condition

Porous treatment of no slip condition is available when **Enable porous media domains** is activated. It controls how the **No Slip** condition on **Wall** boundaries and **Interior Wall** boundaries adjacent to **Porous Medium** should be treated. The options are **Standard no slip formulation** (default) and **Porous slip**. The latter option provides a unified treatment when the porous matrix is fully resolved as well as when it is under resolved ensuring a smooth transition between regions with different resolutions; see No Slip under Wall.

Include Gravity

When the **Include gravity** checkbox is selected, a global **Gravity** feature is shown in the interface model tree, and the buoyancy force is included in the Navier–Stokes equations.

Also, when the **Include gravity** checkbox is selected, the **Use reduced pressure** option changes the pressure formulation from using the total pressure (default) to using the reduced pressure. This option is suitable for configurations where the density changes

are very small; otherwise, the default formulation can be used. For more information, see Gravity.

	Natural convection is induced by variations in magnitude of the buoyancy force that is defined from the density. For incompressible flow, the density is constant; hence the buoyancy force is homogeneous and natural convection cannot be modeled. Nevertheless, using the **Nonisothermal Flow** multiphysics coupling, the buoyancy force is defined using the thermal expansion coefficient and the temperature. Hence, in this case natural convection is accounted for, following the Boussinesq approximation.

Use Shallow Channel Approximation

For 2D components, selecting the **Use shallow channel approximation** checkbox enables modeling of fluid flow in shallow channels in microfluidics applications. Such channels often have an almost rectangular cross section where the **Channel thickness** d_z is much smaller than the channel width. Simple 2D components often fail to give correct results for this type of problems because they exclude the boundaries that have the greatest effect on the flow. The shallow channel approximation takes the effect of these boundaries into account by adding a drag term as a volume force to the momentum equation. The form of this term is

$$\mathbf{F}_\mu = -12\frac{\mu\mathbf{u}}{d_z^{\,2}} \tag{3-1}$$

where μ is the fluid's dynamic viscosity, $\mathbf{u}$ is the velocity field, and d_z is the channel thickness. This term represents the resistance that the parallel boundaries impose on the flow; however, it does not account for any changes in velocity due to variations in the cross-sectional area of the channel.

Reference Values

Reference values are global quantities used to evaluate the density of the fluid when the **Incompressible flow** or the **Weakly compressible flow** option is selected.

Reference pressure level There are generally two ways to include the pressure in fluid flow computations: either to use the absolute pressure $p_A = p + p_{\text{ref}}$, or the gauge pressure p. When p_{ref} is nonzero, the physics interface solves for the gauge pressure whereas material properties are evaluated using the absolute pressure. The reference pressure level is also used to define the reference density.

Reference temperature The reference temperature is used to define the reference density.

Reference position When **Include gravity** is selected, the reference position can be defined. It corresponds to the location where the total pressure (that includes the hydrostatic pressure) is equal to the **Reference pressure level**.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface — the **Velocity field** $\mathbf{u}$ and its components, and the **Pressure** p.

If required, the names of the field, component, and dependent variable can be edited. Editing the name of a scalar dependent variable changes both its field name and the dependent variable name. If a new field name coincides with the name of another field of the same type, the fields share degrees of freedom and dependent variable names. A new field name must not coincide with the name of a field of another type or with a component name belonging to some other field. Component names must be unique within a model except when two fields share a common field name.

CONSISTENT STABILIZATION

To enable this section, click the **Show More Options** button ( ) and select **Stabilization** in the **Show More Options** dialog.

There are two *consistent stabilization methods*: **Streamline diffusion** and **Crosswind diffusion**. Usually, both checkboxes for these methods are selected by default and should remain selected for optimal performance. Consistent stabilization methods do not perturb the original transport equation. Streamline diffusion must be selected when using equal-order interpolation for pressure and velocity.

Select the **Use dynamic subgrid time scale** checkbox to estimate the influence of temporal variations in the velocity field, instead of using the inverse time step, in the consistent stabilization terms. This checkbox is selected by default

Select the **Limit small time steps effect on stabilization time scale** checkbox to prevent loss of stabilization at small time steps.

INCONSISTENT STABILIZATION

To enable this section, click the **Show More Options** button ( ) and select **Stabilization** in the **Show More Options** dialog.

There is usually just one *inconsistent stabilization method* — **Isotropic diffusion**. This method is equivalent to adding a term to the diffusion coefficient in order to dampen

the effect of oscillations by making the system somewhat less dominated by convection. If possible, minimize the use of the inconsistent stabilization method because by using it you no longer solve the original problem. By default, the **Isotropic diffusion** checkbox is not selected because this type of stabilization adds artificial diffusion and affects the accuracy of the original problem. However, this option can be used to get a good initial guess for underresolved problems.

If required, select the **Isotropic diffusion** checkbox and enter a **Tuning parameter** δ_{id} as a scalar positive value. The default value is 0.25 (a reasonable value to start with is roughly 0.5 divided by the element order). A higher value adds more isotropic diffusion.

- Numerical Stability — Stabilization Techniques for Fluid Flow

ADVANCED SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog. Normally these settings do not need to be changed.

The **Use pseudo time stepping for stationary equation form** is per default set to **Automatic from physics**. This option can add pseudo time derivatives to the equation when the **Stationary equation** form is used in order to speed up convergence. Pseudo time stepping is triggered when the Laminar Flow interface is selected in some multiphysics coupling features. Set **Automatic from physics** to **On** to apply pseudo time stepping also for laminar flows. Set it to **Off** to disable pseudo time stepping completely.

When **Use pseudo time stepping for stationary equation form** is set to **Automatic from physics** or **On**, a **CFL number expression** should also be defined. For the default **Automatic** option, the local CFL number (from the Courant–Friedrichs–Lewy condition) is determined by a PID regulator.

The **Use Block Navier-Stokes preconditioner** checkbox under **Linear solver** is available when the **Compressibility** option is set to **Incompressible flow**. When this checkbox is selected, the default solver for time-dependent study steps will use the Block Navier–Stokes preconditioner in iterative solvers for the velocity and pressure. Using this

preconditioner may result in shorter solution times for large time dependent problems with high Reynolds numbers.

- Pseudo Time Stepping for Laminar Flow Models
- Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow
- Theory for the Single-Phase Flow Interfaces
- Block Navier–Stokes in the *COMSOL Multiphysics Reference Manual*.

DISCRETIZATION

The default discretization for Laminar Flow is **P1+P1** elements — that is, piecewise linear interpolation for velocity and pressure. This is suitable for most flow problems.

Some higher-order interpolations are also available, and they can be cost-effective options to obtain high accuracy for flows with low Reynolds numbers.

The **P2+P2** and **P3+P3** options, the equal-order interpolation options, are the preferred higher-order options because they have higher numerical accuracy than the mixed-order options **P2+P1** and **P3+P2**. The equal-order interpolation options do, however, require streamline diffusion to be active.

Flow Past a Cylinder: Application Library path
COMSOL_Multiphysics/Fluid_Dynamics/cylinder_flow

Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow

The following nodes, listed in alphabetical order, are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or by right-clicking to access the context menu (all users).

- Boundary Stress
- Free Surface[2]
- Flow Continuity
- Fluid-Fluid Interface[2]
- Fluid Properties
- Gravity
- Initial Values
- Inlet
- Interior Wall
- Line Mass Source[1]
- Open Boundary
- Outlet
- Periodic Flow Condition
- Point Mass Source[1]
- Porous Interface
- Pressure Point Constraint
- Symmetry
- Volume Force
- Wall

[1] A feature that may require an additional license

[2] See documentation for The Laminar Two-Phase Flow, Moving Mesh Interface

	For 2D axisymmetric components, COMSOL Multiphysics takes the axial symmetry boundaries (at $r = 0$) into account and adds an **Axial Symmetry** node that is valid on the axial symmetry boundaries only.

In the *COMSOL Multiphysics Reference Manual*, see Table 2-4 for links to common sections and Table 2-5 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

	For a detailed overview of the functionality available in each product, visit https://www.comsol.com/products/specifications/

Fluid Properties

The **Fluid Properties** node adds the momentum and continuity equations solved by the physics interface, except for volume forces, which are added by the Volume Force feature. The node also provides an interface for defining the material properties of the fluid.

MODEL INPUTS

Fluid properties, such as density and viscosity, can be defined through user inputs, variables, or by selecting a material. For the latter option, additional inputs, for example temperature or pressure, may be required to define these properties.

Temperature

By default, the **Temperature** model input is set to **Common model input**, and the temperature is controlled from Default Model Inputs under **Global Definitions** or by a locally defined Model Input. If a Heat Transfer interface is included in the component, it controls the temperature **Common model input**. Alternatively, the temperature field can be selected from another physics interface. All physics interfaces have their own tags (**Name**). For example, if a Heat Transfer in Fluids interface is included in the component, the **Temperature (ht)** option is available for T.

You can also select **User defined** from the **Temperature** model input in order to manually prescribe T.

Absolute Pressure

This input appears when a material requires the absolute pressure as a model input. The absolute pressure is used to evaluate material properties, but it also relates to the value of the calculated pressure field. There are generally two ways to calculate the pressure when describing fluid flow: either to solve for the absolute pressure or for a pressure (often denoted gauge pressure) that relates to the absolute pressure through a reference pressure.

The choice of pressure variable depends on the system of equations being solved. For example, in a unidirectional incompressible flow problem, the pressure drop over the modeled domain is probably many orders of magnitude smaller than the atmospheric pressure, which, when included, may reduce the stability and convergence properties of the solver. In other cases, such as when the pressure is part of an expression for the gas volume or the diffusion coefficients, it may be more convenient to solve for the absolute pressure.

The default **Absolute pressure** p_A is $p + p_{\text{ref}}$, where p is the dependent pressure variable from the Navier–Stokes or RANS equations, and p_{ref} is from the user input defined at the physics interface level. When p_{ref} is nonzero, the physics interface solves for a gauge pressure. If the pressure field instead is an absolute pressure field, p_{ref} should be set to 0.

The **Absolute pressure** field can be edited by clicking **Make All Model Inputs Editable** ( ) and entering the desired value in the input field.

	Model Inputs and Multiphysics Couplings in the *COMSOL Multiphysics Reference Manual*

FLUID PROPERTIES

Density

The density can either be specified by a material, or by a **User defined** expression. The density in a material can depend on temperature and pressure, and these dependencies are automatically replaced by p_{ref} for weakly compressible flows and p_{ref} and T_{ref} for incompressible flows (as specified by the **Compressibility** setting at the physics interface level). If density variations with respect to pressure are to be included in the computations, **Compressibility** must be set to compressible. Any dependencies in the density on quantities other than temperature and pressure must be consistent with the **Compressibility** setting at the interface level.

Constitutive Relation

For laminar flow, the **Specify dynamic viscosity** (default) and **Inelastic non-Newtonian** options are available. Use the default option to either get the dynamic viscosity from a material, or to add a user defined expression. The **Inelastic non-Newtonian** option includes several inelastic non-Newtonian models for the relationship between the shear stress and shear rate.

If the **Specify dynamic viscosity** option is selected, an inelastic non-Newtonian model can be selected by adding the corresponding **Material Properties** group as a subnode to a material node.

Dynamic Viscosity

The **Dynamic viscosity** μ describes the relationship between the shear rate and the shear stresses in a fluid. Intuitively, water and air have low viscosities, and substances often described as thick (such as oil) have higher viscosities.

Inelastic Non-Newtonian

Non-Newtonian fluids are encountered in everyday life and in a wide range of the industrial processes. Examples of non-Newtonian fluids include yogurt, paper pulp, and polymer suspensions. Such fluids have a nonlinear relationship between the shear stress and the share rate. The following inelastic non-Newtonian models are available: Power law, Carreau, Bingham–Papanastasiou, Herschel–Bulkley–Papanastasiou and Casson–Papanastasiou.

The following parameters are required for the **Power law**:

- **Fluid consistency coefficient** m
- **Flow behavior index** n
- **Lower shear rate limit** $\dot{\gamma}_{\mathrm{min}}$
- **Reference shear rate** $\dot{\gamma}_{\mathrm{ref}}$

For the **Carreau model**, the following parameters are required:

- **Zero shear rate viscosity** μ_0
- **Infinite shear rate viscosity** μ_{inf}
- **Relaxation time** λ
- **Power index** n

For the **Bingham–Papanastasiou model**, the following parameters are required:

- **Plastic viscosity** μ_{p}
- **Yield stress** τ_{y}
- **Model parameter** m_{p}

For the **Herschel–Bulkley–Papanastasiou model**, the following parameters are required:

- **Fluid consistency coefficient** m
- **Flow behavior index** n
- **Yield stress** τ_{y}
- **Reference shear rate** $\dot{\gamma}_{\mathrm{ref}}$
- **Model parameter** m_{p}

For the **Casson–Papanastasiou model**, the following parameters are required:

- **Plastic viscosity** μ_{p}

- **Yield stress** τ_y
- **Model parameter** m_p

The default values for the parameters are listed in Table 3-1.

TABLE 3-1: DEFAULT VALUES FOR THE INELASTIC NON-NEWTONIAN MODELS.

NAME	UNIT	VARIABLE	DEFAULT VALUE
Fluid consistency coefficient	Pa·s	m	0.001
Flow behavior index / Power index	Dimensionless	n	1
Flow shear rate limit	s^{-1}	$\dot{\gamma}_{min}$	0.01
Reference shear rate	s^{-1}	$\dot{\gamma}_{ref}$	1
Zero shear rate viscosity	Pa·s	μ_0	0.001
Infinite shear rate viscosity	Pa·s	μ_{inf}	0
Relaxation time	s	λ	0
Plastic viscosity	Pa·s	μ_p	0.001
Yield stress	N/m^2	τ_y	0
Model parameter	s	m_p	10

- Non-Newtonian Flow in the *CFD Module User's Guide*

Volume Force

The **Volume Force** node specifies the volume force $\mathbf{F}$ on the right-hand side of the momentum equation.

$$\rho\frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot\left[-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right] + \mathbf{F}$$

If several volume-force nodes are added to the same domain, then the sum of all contributions are added to the momentum equation.

Initial Values

The initial values serve as initial conditions for a transient simulation or as an initial guess for a nonlinear solver in a stationary simulation. Note that for a transient

compressible-flow simulation employing a material for which the density depends on the pressure (such as air), discontinuities in the initial values trigger pressure waves even when the Mach number is small. The pressure waves must be resolved and this puts a restriction on the time step.

INITIAL VALUES

Initial values or expressions should be specified for the **Velocity field** $\mathbf{u}$ and the **Pressure** p.

When **Include gravity** is selected and **Use reduced pressure** not selected in the interface **Physical model** section, the **Compensate for hydrostatic pressure approximation** (named **Compensate for hydrostatic pressure** for compressible flows) checkbox is available and selected by default. When it is selected, the hydrostatic pressure is automatically added to the pressure entered in p user input.

Wall

The **Wall** node includes a set of boundary conditions describing fluid-flow conditions at stationary, moving, and leaking walls. For turbulent flow, the description may involve wall functions and asymptotic expressions for certain turbulence variables.

BOUNDARY CONDITION

Select a **Boundary condition** for the wall.

- No Slip
- Slip
- Electroosmotic Velocity
- Slip Velocity
- Slip Velocity
- Leaking Wall
- Navier Slip

No Slip

No slip is the default boundary condition to model solid walls. A no-slip wall is a wall where the fluid velocity relative to the wall velocity is zero. For a stationary wall that means that $\mathbf{u} = 0$.

The option for **Porous treatment of no slip condition** is available when **Enable porous media domains** is activated in the **Physical Model** section in the settings for the main physics interface node. It specifies how **Wall** boundaries and **Interior Wall** boundaries adjacent to porous domains are treated. When **Standard no slip formulation** is chosen,

a common no slip condition is applied on all solid walls. When the default **Porous slip** is chosen, a blending analytic expression is instead applied on the corresponding wall boundaries adjacent to the porous medium domain. It results in a no slip condition in case the porous length scale is fully resolved by the mesh and a slip condition in the opposite limit when the mesh is much coarser than the porous scale. A smooth transition between these limits is ensured. Note that the interpretation and usage of nonzero slip at the wall is the same as in the **Navier slip** boundary condition. By default, **Velocity formulation** is on and the treatment is based on an approximate reconstruction of the far-field pressure gradient using the slip velocity at the wall. If the **Pressure-gradient formulation** is chosen, the local pressure gradient at the wall is employed.

Slip

The **Slip** option prescribes a no-penetration condition, $\mathbf{u}\cdot\mathbf{n} = 0$. It is implicitly assumed that there are no viscous effects at the slip wall and hence, no boundary layer develops. From a modeling point of view, this can be a reasonable approximation if the main effect of the wall is to prevent fluid from leaving the domain.

Electroosmotic Velocity

When an electric field drives a flow along the boundary, the components for the **Electric field** $\mathbf{E}$ along with the **Electroosmotic mobility** μ_{eo} should be defined. The **Built-in expression** for the **Electroosmotic mobility** requires values or expressions for the **Zeta potential** ζ and the **Relative permittivity** ε_{r}.

Slip Velocity

In the microscale range, the flow condition at a boundary is seldom strictly no slip or slip. Instead, the boundary condition is something in between, and there is a **Slip velocity** at the boundary. Two phenomena account for this velocity: noncontinuum effects and the flow induced by a thermal gradient along the boundary.

When the **Use viscous slip** checkbox is selected, the default **Slip length** L_{s} is **User defined**. Another value or expression may be entered if the default value is not applicable. For **Maxwell's model** values or expressions for the **Tangential momentum accommodation coefficient** a_{v} and the **Mean free path** λ should be specified. Tangential accommodation coefficients are typically in the range of 0.85 to 1.0 and can be found in G. Kariadakis, A. Beskok, and N. Aluru, *Microflows and Nanoflows*, Springer Science and Business Media, 2005.

When the **Use thermal creep** checkbox is selected, a thermal creep contribution with **Thermal slip coefficient** σ_T is activated. Thermal slip coefficients are typically between

0.3 and 1.0 and can be found in G. Kariadakis, A. Beskok, and N. Aluru, *Microflows and Nanoflows*, Springer Science and Business Media, 2005.

Leaking Wall

This boundary condition may be used to simulate a wall where fluid is leaking into or leaving the domain with the velocity $\mathbf{u} = \mathbf{u}_l$ through a perforated wall. The components of the **Fluid velocity** $\mathbf{u}_l$ on the leaking wall should be specified.

Navier Slip

This boundary condition enforces no-penetration at the wall, $\mathbf{u} \cdot \mathbf{n}_{\text{wall}} = 0$, and adds a tangential stress

$$\mathbf{K}_{\text{nt}} = -\frac{\mu}{\beta}\mathbf{u}_{\text{slip}}$$

where $\mathbf{K}_{\text{nt}} = \mathbf{K}_{\text{n}} - (\mathbf{K}_{\text{n}} \cdot \mathbf{n}_{\text{wall}})\mathbf{n}_{\text{wall}}$, $\mathbf{K}_{\text{n}} = \mathbf{K}\mathbf{n}_{\text{wall}}$, and $\mathbf{K}$ is the viscous stress tensor. β is a slip length, and $\mathbf{u}_{\text{slip}} = \mathbf{u} - (\mathbf{u} \cdot \mathbf{n}_{\text{wall}})\mathbf{n}_{\text{wall}}$ is the velocity tangential to the wall.

The **Slip length** setting is per default set to **Factor of minimum element length**. The slip length β is then defined as $\beta = f_{\text{h}}h_{\text{min}}$, where h_{min} is the smallest element side and f_{h} is a user input. Select **User defined** from the **Slip length** selection list in order to manually prescribe β (SI unit: m).

In cases where the wall movement is nonzero, select the **Account for the translational wall velocity of the wall in the friction force** checkbox to use $\mathbf{u} - \mathbf{u}_{\text{bnd}} - ((\mathbf{u} - \mathbf{u}_{\text{bnd}}) \cdot \mathbf{n}_{\text{wall}})\mathbf{n}_{\text{wall}}$ instead of $\mathbf{u}_{\text{slip}}$ in the friction force.

The Navier slip option is not available when selecting a turbulence model.

WALL MOVEMENT

This section contains controls to describe the wall movement relative to the lab (or spatial) frame.

The **Translational velocity** setting controls the translational wall velocity, $\mathbf{u}_{\text{tr}}$. The list is per default set to **Automatic from frame**. The physics automatically detects if the spatial frame moves. This can for example happen if an ALE interface is present in the model component. If there is no movement $\mathbf{u}_{\text{tr}} = \mathbf{0}$. If the frame moves, $\mathbf{u}_{\text{tr}}$ becomes equal to the frame movement. $\mathbf{u}_{\text{tr}}$ is accounted for in the actual boundary condition prescribed in the **Boundary condition** section.

Select **Zero (Fixed wall)** from **Translational velocity** selection list to prescribe $\mathbf{u}_{\text{tr}} = \mathbf{0}$.

Select **Manual** from **Translational velocity** selection list in order to manually prescribe **Velocity of moving wall**, $\mathbf{u}_{\text{tr}}$. This can for example be used to model an oscillating wall

where the magnitude of the oscillations are very small compared to the rest of the model. Specifying translational velocity manually does not automatically cause the associated wall to move. An additional Moving Mesh node needs to be added from Definitions to physically track the wall movement in the spatial reference frame.

The **Sliding wall** option is appropriate if the wall behaves like a conveyor belt with the surface sliding in a tangential direction. A velocity is prescribed at the wall and the boundary itself does not have to actually move relative to the reference frame.

- For 3D components, values or expressions for the **Velocity of sliding wall** $\mathbf{u}_w$ should be specified. If the velocity vector entered is not in the plane of the wall, COMSOL Multiphysics projects it onto the tangential direction. Its magnitude is adjusted to be the same as the magnitude of the vector entered.
- For 2D components, the tangential direction is unambiguously defined by the direction of the boundary. For this reason, the sliding wall boundary condition has different definitions in different space dimensions. A single entry for the **Velocity of the tangentially moving wall** U_w should be specified in 2D.

CONSTRAINT SETTINGS

This section is displayed by clicking the **Show More Options** button ( ) and selecting **Advanced Physics Options** in the **Show More Options** dialog. The **Constraints** settings can be set to **Automatic**, **Pointwise constraints**, **Nitsche constraints**, or **Weak constraints**. **Mixed constraints** can be selected when imposing a no slip condition exactly.

Depending on the constraint method selected, the following settings are available:

- **Apply reaction terms on** can be set to **Individual dependent variables** (default) or **All physics (symmetric)**. This setting is not available when **Nitsche constraints** or, for the **Slip Flow (slpf)** interface, **Weak constraints** is selected.
- Select **Elemental** (default) or **Nodal** under **Constraint method**. This setting is not available for **Nitsche constraints** or **Weak constraints**.

	• Theory for the Wall Boundary Condition • The Moving Mesh Interface in the *COMSOL Multiphysics Reference Manual*

Inlet

This condition should be used on boundaries for which there is a net flow into the domain. To obtain a numerically well-posed problem, it is advisable to also consider the Outlet conditions when specifying an Inlet condition. For example, if the pressure is specified at the outlet, the velocity may be specified at the inlet, and vice versa. Specifying the velocity vector at both the inlet and the outlet may cause convergence difficulties.

BOUNDARY CONDITION

The available **Boundary condition** options for an inlet are **Velocity, Fully developed flow**, **Mass flow**, and **Pressure**. After selecting a **Boundary Condition** from the list, a section with the same or a similar name displays underneath. For example, if **Velocity** is selected, a **Velocity** section, where further settings are defined, is displayed.

VELOCITY

The **Normal inflow velocity** is specified as $\mathbf{u} = -\mathbf{n}U_0$, where $\mathbf{n}$ is the boundary normal pointing out of the domain and U_0 is the normal inflow speed.

The **Velocity field** option sets the velocity vector to $\mathbf{u} = \mathbf{u}_0$. The components of the inlet velocity vector $\mathbf{u}_0$ should be defined for this choice.

PRESSURE CONDITIONS

This option specifies the normal stress, which in most cases is approximately equal to the pressure.

- For incompressible flow, the **Pressure** list has two options, **Static** and **Total**. For weakly compressible and compressible flow, the static pressure should be specified in the text field.
  - If **Pressure** is **Static**, and the reference pressure p_{ref}, defined at the physics interface level, is equal to 0, the value of the pressure p_0, at the boundary, is the absolute pressure. Otherwise, p_0 is the relative pressure at the boundary.
  - If **Pressure** is **Total**, the **Average** checkbox is available and cleared by default to prescribe the total pressure pointwise. If it is selected, the averaged total pressure is imposed in the weak forms instead.

  When **Include gravity** is selected and **Use reduced pressure** not selected in the interface **Physical model** section, the **Compensate for hydrostatic pressure approximation** (named **Compensate for hydrostatic pressure** for incompressible flows) checkbox is

available and selected by default. When it is selected, the hydrostatic pressure is automatically added to the pressure entered in p_0 user input.

- The **Suppress backflow** option adjusts the inlet pressure locally in order to reduce the amount of fluid exiting the domain through the boundary. If you clear the suppress backflow option, the inlet boundary can become an outlet depending on the pressure field in the rest of the domain.
- **Flow direction** controls in which direction the fluid enters the domain.
  - For **Normal flow**, it prescribes zero tangential velocity component.
  - For **User defined**, an **Inflow velocity direction** $\mathbf{d_u}$ (dimensionless) should be specified. The magnitude of $\mathbf{d_u}$ does not matter, only the direction. $\mathbf{d_u}$ must point into the domain.

MASS FLOW

The mass flow at an inlet can be specified by the **Mass flow rate**, the **Pointwise mass flux**, the **Standard flow rate**, or the **Standard flow rate (SCCM)**.

The **Apply condition on each disjoint selection separately** checkbox is selected per default. When this setting is selected, the mass flow condition is applied separately on each disjoint selection. If this option is not selected, the condition is applied over the whole feature selection. The **Apply condition on each disjoint selection separately** should be disabled only if the flow conditions are known to be identical on each disjoint boundary.

Mass Flow Rate

The **Mass flow rate** option sets the integrated mass flow over the boundary selection, the **Normal mass flow rate** to a specific value, m. The mass flow is assumed to be parallel to the boundary normal, and the tangential flow velocity is set to zero.

For 2D components, the **Channel thickness** d_{bc} is used to define the area across which the mass flow occurs. This setting is not applied to the whole model. Line or surface integrals of the mass flow over the boundary evaluated during postprocessing or used in integration coupling operators do not include this scaling automatically. Such results should be appropriately scaled when comparing them with the specified mass flow.

Pointwise Mass Flux

The **Pointwise mass flux** sets the mass flow parallel to the boundary normal. The tangential flow velocity is set to zero. The mass flux is a model input, which means that COMSOL Multiphysics can take its value from another physics interface when

available. When **User defined** is selected a value or function M_f should be specified for the **Mass flux**.

Standard Flow Rate

The **Standard flow rate** Q_{sv} sets a standard volumetric flow rate, according to the SEMI standard E12-0303. The mass flow rate is specified as the volumetric flow rate of a gas at standard density — the **Mean molar mass** M_n divided by a **Standard molar volume** V_{m} (that is, the volume of one mole of a perfect gas at standard pressure and standard temperature). The flow occurs across the whole boundary in the direction of the boundary normal and is computed by a surface (3D) or line (2D) integral. The tangential flow velocity is set to zero.

The standard density can be defined directly, or by specifying a standard pressure and temperature, in which case the ideal gas law is assumed. The options in the **Standard flow rate defined by** list are:

- **Standard density**, for which the **Standard molar volume** V_{m} should be specified.
- **Standard pressure and temperature**, for which the **Standard pressure** P_{st} and the **Standard temperature** T_{st} should be defined.

For 2D components, the **Channel thickness** d_{bc} is used to define the area across which the mass flow occurs. This setting is not applied to the whole model. Line or surface integrals of the mass flow over the boundary evaluated during postprocessing or used in integration coupling operators do not include this scaling automatically. Such results should be appropriately scaled when comparing them with the specified mass flow.

Standard Flow Rate (SCCM)

The **Standard flow rate (SCCM)** boundary condition is equivalent to the **Standard flow rate** boundary condition, except that the flow rate is entered directly in SCCMs (standard cubic centimeters per minute) without the requirement to specify units. Here, the dimensionless **Number of SCCM units** Q_{sccm} should be specified.

FULLY DEVELOPED FLOW

The **Fully developed flow** option adds contributions to the inflow boundary, which force the flow toward the solution for a fully developed channel flow. The channel can be thought of as a virtual extrusion of the inlet cross section. The inlet boundary must hence be flat in order for the fully developed flow condition to work properly. In 2D axisymmetric models, the inlet normal must be parallel to the symmetry axis.

Select an option to control the flow rate at the inlet:

- **Average velocity**, U_{av}.

- **Flow rate**, V_0. Two-dimensional models also require an **Entrance thickness**, D_z, which is the out-of-plane thickness of the extruded entrance channel.
- **Average pressure**, P_{av}. Note that P_{av} is the average pressure on the inflow boundary.

The **Apply condition on each disjoint selection separately** checkbox is selected per default. When this setting is selected, the fully developed flow condition is applied separately on each disjoint selection. If this option is not selected, the condition is applied over the whole feature selection. The **Apply condition on each disjoint selection separately** should be disabled only if the flow conditions are known to be identical on each disjoint boundary.

The fully developed flow condition requires any volume force to be approximately aligned with the normal of the inlet boundary. The exception is gravity when the **Include gravity** setting is selected in the physics interface settings. Unless **Use reduced pressure** is also selected, an option to **Compensate for hydrostatic pressure** or **Compensate for hydrostatic pressure approximation** becomes available. It is selected per default and should only be deselected if the inlet normal is aligned with the gravity force and you want to specify an average pressure that includes the hydrostatic pressure.

CONSTRAINT SETTINGS

This section is displayed by clicking the **Show** button ( ) and selecting **Advanced Physics Options**.

	• Prescribing Inlet and Outlet Conditions • Normal Stress Boundary Condition

	Fully Developed Flow (Inlet)

Outlet

This condition should be used on boundaries for which there is a net outflow from the domain. To obtain a numerically well-posed problem, it is advisable to also consider the Inlet conditions when specifying an Outlet condition. For example, if the velocity is specified at the inlet, the pressure may be specified at the outlet, and vice versa. Specifying the velocity vector at both the inlet and the outlet may cause convergence difficulties. Selecting appropriate outlet conditions for the Navier–Stokes equations is

a nontrivial task. Generally, if there is something interesting happening at an outflow boundary, the computational domain should be extended to include this phenomenon.

BOUNDARY CONDITION

The available **Boundary condition** options for an outlet are **Pressure, Velocity, Fully developed flow**, and **Mass flow**.

PRESSURE CONDITIONS

This option specifies the normal stress, which in most cases is approximately equal to the pressure. The tangential stress component is set to zero.

- For incompressible flow, the **Pressure** list has two options, **Static** and **Total**. For weakly compressible and compressible flow, the static pressure should be specified in the text field.
  - If **Pressure** is **Static**, and the reference pressure p_{ref}, defined at the physics interface level, is equal to 0, the value of the pressure p_0, at the boundary, is the absolute pressure. Otherwise, p_0 is the relative pressure at the boundary.
  - If **Pressure** is **Total**, the **Average** checkbox is available and selected by default to prescribed the averaged total pressure in the weak forms. If it is cleared, the total pressure is imposed pointwise.

When **Include gravity** is selected and **Use reduced pressure** not selected in the interface **Physical model** section, the **Compensate for hydrostatic pressure approximation** (named **Compensate for hydrostatic pressure** for incompressible flows) checkbox is available and selected by default. When it is selected, the hydrostatic pressure is automatically added to the pressure entered in p_0 user input.

- The **Normal flow** option changes the no tangential stress condition to a no tangential velocity condition. This forces the flow to exit (or enter) the domain perpendicularly to the outlet boundary.
- The **Suppress backflow** checkbox is selected by default. This option adjusts the outlet pressure in order to reduce the amount of fluid entering the domain through the boundary.

VELOCITY

See the **Inlet** node Velocity section for the settings.

FULLY DEVELOPED FLOW

This boundary condition is applicable when the flow exits the domain into a long pipe or channel, at the end of which a flow profile is fully developed.

The channel can be thought of as a virtual extrusion of the outlet cross section. The outlet boundary must hence be flat in order for the fully developed flow condition to work properly. In 2D axisymmetric models, the outlet normal must be parallel to the symmetry axis.

Select an option to control the flow rate at the outlet:

- **Average velocity**, U_{av}.
- **Flow rate**, V_0. Two-dimensional models also require an **Entrance thickness**, D_z, which is the out-of-plane thickness of the extruded entrance channel.
- **Average pressure**, P_{av}. Observe that P_{av} is the average pressure on the outflow.

The **Apply condition on each disjoint selection separately** checkbox is selected per default. When this setting is selected, the fully developed flow condition is applied separately on each disjoint selection. If this option is not selected, the condition is applied over the whole feature selection. The **Apply condition on each disjoint selection separately** should be disabled only if the flow conditions are known to be identical on each disjoint boundary.

The fully developed flow condition requires any volume force to be approximately aligned with the normal of the outlet boundary. The exception is gravity when the **Include gravity** setting is selected in the physics interface settings. Unless **Use reduced pressure** is also selected, an option to **Compensate for hydrostatic pressure** or **Compensate for hydrostatic pressure approximation** becomes available. It is selected per default and should only be deselected if the outlet normal is aligned with the gravity force and you want to specify an average pressure that includes the hydrostatic pressure.

MASS FLOW

See the **Inlet** node Mass Flow section for the settings.

CONSTRAINT SETTINGS

This section is displayed by clicking the **Show** button ( ) and selecting **Advanced Physics Options**.

	Prescribing Inlet and Outlet Conditions

	Fully Developed Flow (Outlet)

Symmetry

This node provides a boundary condition for symmetry boundaries. It should only be used when the geometry and expected solution have mirror symmetry. By using symmetries in a model its size can be reduced by one-half or more, making this an efficient tool for solving large problems.

The **Symmetry** boundary condition prescribes no penetration and vanishing shear stresses. The boundary condition is a combination of a Dirichlet condition and a Neumann condition:

$$\mathbf{u}\cdot\mathbf{n} = \mathbf{0}, \qquad \left(-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right)\mathbf{n} = \mathbf{0}$$

$$\mathbf{u}\cdot\mathbf{n} = \mathbf{0}, \qquad (-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^{\mathrm{T}}))\mathbf{n} = \mathbf{0}$$

for the compressible and incompressible formulations. The Dirichlet condition takes precedence over the Neumann condition, and the above equations are equivalent to the following equation for both the compressible and incompressible formulations:

$$\mathbf{u}\cdot\mathbf{n} = \mathbf{0}, \qquad \mathbf{K} - (\mathbf{K}\cdot\mathbf{n})\mathbf{n} = \mathbf{0}$$
$$\mathbf{K} = \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^{\mathrm{T}})\mathbf{n}$$

BOUNDARY SELECTION

For 2D axial symmetry, a boundary condition does not need to be defined for the symmetry axis at $r = 0$. The software automatically provides a condition that prescribes $u_r = 0$ and vanishing stresses in the z direction and adds an **Axial Symmetry** node that implements these conditions on the axial symmetry boundaries only.

CONSTRAINT SETTINGS

This section is displayed by clicking the **Show** button ( ) and selecting **Advanced Physics Options**.

Open Boundary

The **Open Boundary** condition describes boundaries in contact with a large volume of fluid. Fluid can both enter and leave the domain on boundaries with this type of condition.

BOUNDARY CONDITIONS

The **Boundary condition** options for open boundaries are **Normal stress** and **No viscous stress**.

Normal Stress

The **Normal stress** f_0 condition implicitly imposes $p \approx \mathrm{f}_0$.

When **Include gravity** is selected and **Use reduced pressure** not selected in the interface **Physical model** section, the **Compensate for hydrostatic pressure approximation** (named **Compensate for hydrostatic pressure** for incompressible flows) checkbox is available and selected by default. When it is selected, the hydrostatic pressure is automatically added to the pressure entered in f_0 user input.

No Viscous Stress

The **No Viscous Stress** condition specifies vanishing viscous stress on the boundary. This condition does not provide sufficient information to fully specify the flow at the open boundary and must at least be combined with pressure constraints at adjacent points.

The **No viscous stress** condition prescribes:

$$\left(\mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right)\mathbf{n} = \mathbf{0}$$

$$\mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)\mathbf{n} = \mathbf{0}$$

for the compressible and the incompressible formulations. This condition can be useful in some situations because it does not impose any constraint on the pressure. A typical example is a model with volume forces that give rise to pressure gradients that are hard to prescribe in advance. To make the model numerically stable, this boundary condition should be combined with a point constraint on the pressure.

Boundary Stress

The **Boundary Stress** node adds a boundary condition that represents a general class of conditions also known as traction boundary conditions.

BOUNDARY CONDITION

The **Boundary condition** options for the boundary stress are **General stress**, **Normal stress**, and **Normal stress, normal flow**.

General Stress

When **General stress** is selected, the components for the **Stress** $\mathbf{F}$ should be specified. The total stress on the boundary is set equal to the given stress $\mathbf{F}$:

$$\left(-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)-\frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right)\mathbf{n} = \mathbf{F}$$

$$(-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T))\mathbf{n} = \mathbf{F}$$

for the compressible and the incompressible formulations.

This boundary condition implicitly sets a constraint on the pressure that for 2D flows is

$$p = 2\mu\frac{\partial u_n}{\partial n}-\mathbf{n}\cdot\mathbf{F} \tag{3-2}$$

If $\partial u_n/\partial n$ is small, Equation 3-2 states that $p \approx -\mathbf{n}\cdot\mathbf{F}$.

Normal Stress

Normal Stress is described for the Open Boundary node.

Normal Stress, Normal Flow

For **Normal stress, normal flow**, the magnitude of the **Normal stress** f_0 should be specified. The tangential velocity is set to zero on the boundary:

$$\mathbf{n}^T\left(-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)-\frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right)\mathbf{n} = -\mathrm{f}_0, \qquad \mathbf{t}\cdot\mathbf{u} = 0$$

$$\mathbf{n}^T(-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T))\mathbf{n} = -\mathrm{f}_0, \qquad \mathbf{t}\cdot\mathbf{u} = 0$$

for the compressible and the incompressible formulations.

This boundary condition implicitly sets a constraint on the pressure that for 2D flows is

$$p = 2\mu\frac{\partial u_n}{\partial n} + \mathrm{f}_0 \tag{3-3}$$

If $\partial u_n/\partial n$ is small, Equation 3-3 states that $p \approx \mathrm{f}_0$.

When **Include gravity** is selected and **Use reduced pressure** not selected in the interface **Physical model** section, the **Compensate for hydrostatic pressure approximation** (named **Compensate for hydrostatic pressure** for incompressible flows) checkbox is available and selected by default. When it is selected, the hydrostatic pressure is automatically added to the pressure entered in f_0 or $p_{\mathrm{hydro}}\mathbf{n}$ is added to $\mathbf{F}$ depending on the selected option.

CONSTRAINT SETTINGS

This section is displayed by clicking the **Show** button (👁) and selecting **Advanced Physics Options**.

If Normal Stress, Normal Flow is selected as the **Boundary condition**, then to **Apply reaction terms on** all dependent variables, the **All physics (symmetric)** option should be selected. Alternatively, the **Individual dependent variables** could be selected to restrict the reaction terms as needed.

Periodic Flow Condition

The **Periodic Flow Condition** splits its selection into a source group and a destination group (the **Destination Selection** section is optional). Fluid that leaves the domain through one of the destination boundaries enters the domain through the corresponding source boundary. This corresponds to a situation where the geometry is a periodic part of a larger geometry. If the boundaries are not parallel to each other, the velocity vector is automatically transformed.

If the boundaries are curved, the orientation of the source must be specified manually (see Orientation of Source).

No input is required when **Compressible flow (Ma<0.3)** is selected for **Compressibility** under the **Physical Model** section for the physics interface. Typically when a periodic boundary condition is used with a compressible flow, the pressure is the same at both boundaries and the flow is driven by a volume force.

BOUNDARY SELECTION

The software usually automatically identifies the boundaries as either source boundaries or destination boundaries, as indicated in the selection list. This works fine for cases like opposing parallel boundaries. In other cases, right-click **Periodic Flow Condition** and select **Manual Destination Selection** to control the destination. By default it contains the selection that COMSOL Multiphysics identifies.

DESTINATION SELECTION

This section is available for specifying the destination boundaries, if needed, when the **Manual Destination Selection** option is selected in the context menu for the **Periodic Flow Condition** node. You can only select destination boundaries from the union of all source and destination boundaries.

FLOW CONDITION

This section is available when **Incompressible flow** is selected for **Compressibility** under the **Physical Model** section for the physics interface.

The **Flow Condition** at the boundary is specified through a value or expression for either the **Pressure difference**, $p_{\mathrm{src}} - p_{\mathrm{dst}}$, or the **Mass flow**, $\dot{m}$. The mass flow option ensures a pressure difference is achieved across the source and destination boundaries. This pressure difference can, for example, drive the fully developed flow in a channel.

To set up a periodic boundary condition, both boundaries must be selected in the **Periodic Flow Condition** node. COMSOL Multiphysics automatically assigns one boundary as the source and the other as the destination. To manually set the destination selection, a **Destination Selection** subnode is available from the context menu (by right-clicking the parent node) or from the **Physics** toolbar, **Attributes** menu. All destination sides must be connected.

ORIENTATION OF SOURCE

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog. For information about the **Orientation of Source** section, see Orientation of Source and Destination in the *COMSOL Multiphysics Reference Manual.*

ORIENTATION OF DESTINATION

This section appears if the setting for **Transform to intermediate map** in the **Orientation of Source** section is changed from the default value, **Automatic**, and **Advanced Physics**

Options is selected in the **Show More Options** dialog. For information about the **Orientation of Destination** section, see Orientation of Source and Destination in the *COMSOL Multiphysics Reference Manual.*

MAPPING BETWEEN SOURCE AND DESTINATION

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog. For information about the **Mapping Between Source and Destination** section, see Mapping Between Source and Destination in the *COMSOL Multiphysics Reference Manual.*

Interior Wall

The **Interior Wall** boundary condition can only be applied on interior boundaries.

It is similar to the Wall boundary condition available on exterior boundaries except that it applies on both sides of an interior boundary. It allows discontinuities (velocity, pressure) across the boundary. The **Interior Wall** boundary condition can be used to avoid meshing thin structures by applying no-slip conditions on interior curves and surfaces instead. Slip conditions and conditions for a moving wall can also be prescribed. It is compatible with laminar and turbulent flow.

BOUNDARY CONDITION

The following **Boundary condition** options are available.

No Slip

The **No slip** condition models solid walls. No slip walls are walls where the fluid velocity relative to the wall is zero. For an interior stationary wall this means that $\mathbf{u} = 0$ on both sides of the wall.

Slip

The **Slip** condition prescribes a no-penetration condition, $\mathbf{u} \cdot \mathbf{n} = 0$. It implicitly assumes that there are no viscous effects on either side of the slip wall and hence, no boundary layer develops. From a modeling point of view, this can be a reasonable approximation if the important effect is to prevent the exchange of fluid between the regions separated by the interior wall.

Navier Slip

The **Navier slip** condition enforces no-penetration at the wall, $\mathbf{u} \cdot \mathbf{n}_{\text{wall}} = 0$, and adds a tangential stress on each side of the wall

$$\mathbf{K}_{nt} = -\frac{\mu}{\beta}\mathbf{u}_{slip}$$

where β is a slip length. For more information, see the **Navier Slip** option in the Wall feature.

WALL MOVEMENT

This section contains controls to describe the wall movement relative to the lab (or spatial) frame.

The **Translational velocity** setting controls the translational wall velocity, $\mathbf{u_{tr}}$. The list is per default set to **Automatic from frame**. The physics automatically detects if the spatial frame moves. This can for example happen if an ALE interface is present in the model component. If there is no movement $\mathbf{u_{tr}} = \mathbf{0}$. If the frame moves, $\mathbf{u_{tr}}$ becomes equal to the frame movement. $\mathbf{u_{tr}}$ is accounted for in the actual boundary condition prescribed in the **Boundary condition** section.

Select **Zero (Fixed wall)** from **Translational velocity** selection list to prescribe $\mathbf{u}_{tr} = \mathbf{0}$.

Select **Manual** from **Translational velocity** selection list in order to manually prescribe **Velocity of moving wall**, $\mathbf{u_{tr}}$. This can for example be used to model an oscillating wall where the magnitude of the oscillations are very small compared to the rest of the model. Specifying translational velocity manually does not automatically cause the associated wall to move. An additional Moving Mesh interface needs to be added to physically track the wall movement in the spatial reference frame.

CONSTRAINT SETTINGS

This section is displayed by clicking the **Show** button ( ) and selecting **Advanced Physics Options**. The **Constraints** settings can be set to **Automatic**, **Pointwise constraints**, or **Nitsche constraints**. **Mixed constraints** can be selected when imposing a no slip condition exactly.

Porous Interface

The **Porous Interface** condition is designed to properly account for a sudden jump in porosity, ε_p, across a boundary between different domains. It describes possible discontinuity of stress across the interface, and also reveals modified behavior of tangential velocity due to boundary layer on the upstream side of the interface. Choose among the following options under the **Continuity conditions**:

- **Velocity and stress** — stress continuity is invoked;

- **Velocity and porosity-corrected stress** (default)— the sum of stress and a contribution due to the inertial term being constant across the interface;
- **Velocity and porosity-corrected stress with loss** — the sum of the stress and a contribution due to the inertial term is lost in the downstream direction.

All three options give continuity of the velocity across the interface in constant-density flows, while in case of a jump in density:

1. give continuity of the mass flux (product of density and normal velocity) and tangential velocity;
2. account for the density-jump correction in the stress condition.

When **Velocity and porosity-corrected stress with loss** is chosen, a **Pressure loss model** needs to be specified. The options are:

- **User-defined loss coefficients** (default). Enter values for **Expansion loss coefficient** and **Contraction loss coefficient**;
- **Borda–Carnot**. Specify **Vena contracta model**.

Vena contracta model allows two options:

- **User defined** (default) — enter value of **Vena contracta coefficient**;
- **Weisbach** — enter values of **Lower limit** and **Exponent**.

Notice that the notions 'expansion' and 'contraction' used in this section correspond not to geometrical changes, but to the variations of the microscopic structure across the interface in the flow direction — increasing or decreasing porosity, ε_p, respectively.

Flow Continuity

The **Flow Continuity** condition is suitable for pairs where the boundaries match; it prescribes that the flow field is continuous across the pair.

The parts of the boundary where a source boundary lacks a corresponding destination boundary and vice versa will get conditions from other boundary conditions under the physics interface acting as fallback boundary conditions on the nonoverlapping parts. By default, the Wall node is used as fallback unless another feature has been selected for the boundary.When the condition is set for pairs adjacent to domains with different porosity ε_p, it imposes conditions identical to the **Porous Interface** feature, which is designed to properly account for a sudden jump in porosity. See the section Porous

Interface above for further details (note that the **Flow Continuity** does not account for the density-jump corrections),

	About Pairs

Pressure Point Constraint

The **Pressure Point Constraint** condition can be used to specify the pressure level. If it is not possible to specify the pressure level using a boundary condition, the pressure level must be set in some other way, for example, by specifying a fixed pressure at a point.

PRESSURE CONSTRAINT

The relative pressure value is set by specifying the **Pressure** p_0. If the reference pressure p_{ref} defined at the physics interface level is equal to zero, p_0 represents the absolute pressure.

When **Include gravity** is selected and **Use reduced pressure** not selected in the interface **Physical model** section, the **Compensate for hydrostatic pressure approximation** (named **Compensate for hydrostatic pressure** for incompressible flows) checkbox is available and selected by default. When it is selected, the hydrostatic pressure is automatically added to the pressure entered in p_0 user input.

CONSTRAINT SETTINGS

This section is displayed by clicking the **Show** button ( ) and selecting **Advanced Physics Options**.

The **Apply reaction terms on** setting is set per default to **Individual dependent variables**. **All physics (symmetric)** cannot be used together with a segregated solver when fluid flow is coupled with Moving Mesh, Level Set, or Phase Field in Fluids.

Point Mass Source

This feature requires at least one of the following licenses: Battery Design Module, CFD Module, Chemical Reaction Engineering Module, Corrosion Module, Electrochemistry Module, Electrodeposition Module, Fuel Cell & Electrolyzer Module, Microfluidics Module, Pipe Flow Module, or Subsurface Flow Module.

The **Point Mass Source** feature models mass flow originating from an infinitely small domain centered around a point.

For the Reacting Flow in Porous Media, Diluted Species interface, which is available with the CFD Module, Chemical Reaction Engineering Module, or Battery Design Module, there are two nodes: one for the fluid flow (**Fluid Point Source**) and one for the species (**Species Point Source**).

SOURCE STRENGTH

The source **Mass flux**, $\dot{q}_{\mathrm{p}}$ should be specified. A positive value results in mass being ejected from the point into the computational domain. A negative value results in mass being removed from the computational domain.

Point sources located on a boundary or on an edge affect the adjacent computational domains. This has the effect, for example, that a point source located on a symmetry plane has twice the given strength.

	Mass Sources for Fluid Flow in the *COMSOL Multiphysics Reference Manual*

Line Mass Source

This feature requires at least one of the following licenses: Battery Design Module, CFD Module, Chemical Reaction Engineering Module, Corrosion Module, Electrochemistry Module, Electrodeposition Module, Fuel Cell & Electrolyzer Module, Microfluidics Module, Pipe Flow Module, or Subsurface Flow Module.

The **Line Mass Source** feature models mass flow originating from a tube region with infinitely small radius.

For the Reacting Flow in Porous Media, Diluted Species interface, which is available with the CFD Module, Chemical Reaction Engineering Module, or Battery Design Module, there are two nodes, one for the fluid flow (**Fluid Line Source**) and one for the species (**Species Line Source**).

SELECTION

The **Line Mass Source** feature is available for all dimensions, but the applicable selection differs between the dimensions.

MODEL DIMENSION	APPLICABLE GEOMETRICAL ENTITY
2D	Points
2D Axisymmetry	Points not on the axis of symmetry
3D	Edges

SOURCE STRENGTH

The source **Mass flux**, $\dot{q}_1$, should be specified. A positive value results in mass being ejected from the line into the computational domain and a negative value means that mass is removed from the computational domain.

Line sources located on a boundary affect the adjacent computational domains. This, for example, has the effect that a line source located on a symmetry plane has twice the given strength.

	Mass Sources for Fluid Flow in the *COMSOL Multiphysics Reference Manual*

Gravity

The **Gravity** global feature is automatically added when **Include gravity** is selected at the interface level in the **Physical Model** settings. It defines the gravity forces from the **Acceleration of gravity** value.

ACCELERATION OF GRAVITY

The **Acceleration of gravity** (SI unit m/s, default value $-g_{\text{const}}\mathbf{e_z}$ in 2D axial symmetry and 3D and $-g_{\text{const}}\mathbf{e_y}$ in 2D) is used to define the gravity forces. It should be a global quantity.

The Potential Flow Interface

In this section

- The Incompressible Potential Flow Interface

The Incompressible Potential Flow Interface

The **Incompressible Potential Flow (ipf)** interface ( ) is used for simulating irrotational, inviscid, and incompressible flow. The main application of the interface is to provide initial solutions for other Single-Phase Flow interfaces.

The equation solved by the Incompressible Potential Flow interface is the Laplace equation for a velocity potential. This can be used to derive both a velocity and static pressure.

The Incompressible Potential Flow interface is available for stationary analyses. The main feature is Fluid Properties, which adds the Laplace equation. The Fluid Properties feature provides an interface for defining the fluid material and its properties used to derive the velocity and pressure. When this physics interface is added, the following default nodes are also added in the **Model Builder**:

- **Fluid Properties**
- **Initial Values**
- **Wall**

Then, from the **Physics** toolbar, add other nodes that implement boundary conditions. You can also right-click **Incompressible Potential Flow** to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is ipf.

PRESSURE

This node specifies **Total pressure** (SI unit: Pa) used to compute the pointwise static pressure from the potential flow solution.

DEPENDENT VARIABLES

This physics interface solves for the **Velocity Potential** ϕ-dependent variable (field).

If required, the names of the field, component, and dependent variable can be edited. Editing the name of a scalar dependent variable changes both its field name and the dependent variable name. If a new field name coincides with the name of another field of the same type, the fields share degrees of freedom and dependent variable names. A new field name must not coincide with the name of a field of another type or with a component name belonging to some other field. Component names must be unique within a model except when two fields share a common field name.

DISCRETIZATION

Select shape function type for the velocity potential. The default setting is **Quadratic**.

	• Domain, Boundary, Point, and Pair Nodes for the Incompressible Potential Flow Interface • Theory for the Incompressible Potential Flow Interface

	Flow Around an Inclined NACA 0012 Airfoil: Application Library path **CFD_Module/Verification_Examples/naca0012_airfoil**

Domain, Boundary, Point, and Pair Nodes for the Incompressible Potential Flow Interface

The Incompressible Potential Flow Interface has the following domain, boundary, and pair nodes:

- Initial Values
- Interior Wall
- Flow Continuity
- Fluid Properties
- Open Boundary
- Periodic Flow Condition (see Periodic Boundary Conditions in the *COMSOL Multiphysics Reference Manual*)
- Potential Point Constraint
- Symmetry
- Velocity
- Wall

[1] Described for the Laminar Flow interface.

	Boundary conditions for axial symmetry boundaries are not required. For the symmetry axis at $r = 0$, the software automatically provides a suitable boundary condition and adds an **Axial Symmetry** node that is valid on the axial symmetry boundaries only.

!	In the *COMSOL Multiphysics Reference Manual* see Table 2-4 for links to common sections and Table 2-5 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Fluid Properties

The **Fluid Properties** node adds the Laplace equation solved by the physics interface. The node also provides an interface for defining the density of the fluid, and builds the velocity and static pressure.

Material Properties

The density can either be specified by a material, or by a **User defined** expression.

Initial Values

Use the **Initial Values** node to define the initial values of the velocity potential variable.

INITIAL VALUES

An initial value or expression should be specified for the **Velocity Potential** ϕ.

Wall

The **Wall** node sets a slip wall condition for the fluid. This prescribes a no-penetration condition, $\mathbf{u}\cdot\mathbf{n} = 0$.

WALL MOVEMENT

This section contains controls to describe the wall movement relative to the lab (or spatial) frame.

The **Normal wall velocity** setting controls the normal wall velocity U_{bnd}. The list is per default set to **Automatic from frame**. The physics automatically detects if the spatial frame moves. This can for example happen if an ALE interface is present in the model component. If there is no movement $U_{bnd} = 0$. If the frame moves, U_{bnd} becomes equal to the frame movement projected on the wall normal. U_{bnd} is accounted for in the actual nonpenetration boundary condition prescribed, so that $\mathbf{u} \cdot \mathbf{n} = U_{bnd}$.

Select **Zero (Fixed wall)** from **Normal wall velocity** selection list to always prescribe $U_{bnd} = 0$.

Velocity

The **Velocity** node sets a normal inflow velocity condition for the fluid. This prescribes a flux condition for the velocity potential, $\nabla\phi \cdot \mathbf{n} = -U_{in}$.

Open Boundary

The **Open Boundary** node sets a normal flow condition for the fluid. The level of ϕ is set to a constant value along the boundary, so that the tangential derivative of ϕ is zero.

OPEN BOUNDARY

The potential level is set by specifying the **Velocity potential** ϕ_{bnd}.

CONSTRAINT SETTINGS

This section is displayed by clicking the **Show** button ( ) and selecting **Advanced Physics Options**.

Symmetry

The **Symmetry** node prescribes a symmetry condition for the velocity potential, $\nabla\phi \cdot \mathbf{n} = 0$.

Potential Point Constraint

The **Potential Point Constraint** node can be used to specify the velocity potential level. If it is not possible to specify the velocity potential level using a boundary condition, the level must be set in some other way, such as specifying a fixed potential at a point.

POTENTIAL POINT CONSTRAINT

The potential level is set by specifying the **Velocity potential** ϕ_p.

CONSTRAINT SETTINGS

This section is displayed by clicking the **Show** button ( ) and selecting **Advanced Physics Options**.

Periodic Flow Condition

The **Periodic Flow Condition** splits its selection into a source group and a destination group (the **Destination Selection** section is optional). Fluid that leaves the domain through one of the destination boundaries enters the domain through the corresponding source boundary. This corresponds to a situation where the geometry is a periodic part of a larger geometry. If the boundaries are not parallel to each other, the velocity vector is automatically transformed.

If the boundaries are curved, the orientation of the source must be specified manually (see Orientation of Source).

OFFSET

The **Offset** at the boundary specifies a value or expression for either the **Velocity potential difference**, $\phi_{src} = -\phi_{dst}$. The offset ensures a gradient of the Velocity potential between the source and destination, so that the velocity is nonzero.

BOUNDARY SELECTION

To set up a periodic boundary condition, both boundaries must be selected in the **Periodic Flow Condition** node. COMSOL Multiphysics automatically assigns one boundary as the source and the other as the destination. To manually set the destination selection, a **Destination Selection** subnode is available from the context menu (by right-clicking the parent node) or from the **Physics** toolbar, **Attributes** menu. All destination sides must be connected.

	The software usually automatically identifies the boundaries as either source boundaries or destination boundaries, as indicated in the selection list. This works fine for cases like opposing parallel boundaries. In other cases, right-click **Periodic Flow Condition** and select **Manual Destination Selection** to control the destination. By default it contains the selection that COMSOL Multiphysics identifies.

DESTINATION SELECTION

This section is available for specifying the destination boundaries, if needed, when the **Manual Destination Selection** option is selected in the context menu for the **Periodic Flow Condition** node. You can only select destination boundaries from the union of all source and destination boundaries.

ORIENTATION OF SOURCE

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog. For information about the **Orientation of Source** section, see Orientation of Source and Destination in the *COMSOL Multiphysics Reference Manual*.

ORIENTATION OF DESTINATION

This section appears if the setting for **Transform to intermediate map** in the **Orientation of Source** section is changed from the default value, **Automatic**, and **Advanced Physics Options** is selected in the **Show More Options** dialog. For information about the **Orientation of Destination** section, see Orientation of Source and Destination in the *COMSOL Multiphysics Reference Manual*.

MAPPING BETWEEN SOURCE AND DESTINATION

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog. For information about the **Mapping**

Between Source and Destination section, see Mapping Between Source and Destination in the *COMSOL Multiphysics Reference Manual*.

Interior Wall

The **Interior Wall** boundary condition can only be applied on interior boundaries.

It is similar to the Wall node available on exterior boundaries except that it applies on both sides of an interior boundary. It allows discontinuities of the velocity potential across the boundary. The **Interior Wall** boundary condition can be used to avoid meshing thin structures by applying a no-penetration condition, $\mathbf{u} \cdot \mathbf{n} = U_{bnd}$, on interior curves and surfaces instead. Slip conditions and conditions for a moving wall can also be prescribed.

WALL MOVEMENT

This section contains controls to describe the wall movement relative to the lab (or spatial) frame.

The **Normal wall velocity** setting controls the normal wall velocity U_{bnd}. The list is per default set to **Automatic from frame**. The physics automatically detects if the spatial frame moves. This can for example happen if an ALE interface is present in the model component. If there is no movement $U_{bnd} = 0$. If the frame moves, U_{bnd} becomes equal to the frame movement projected on the wall normal. U_{bnd} is accounted for in the actual no-penetration boundary condition prescribed, so that $\mathbf{u} \cdot \mathbf{n} = U_{bnd}$.

Select **Zero (Fixed wall)** from **Normal wall velocity** selection list to always prescribe $U_{bnd} = 0$.

Flow Continuity

The **Continuity** condition is suitable for pairs where the boundaries match; it prescribes that the velocity potential variable is continuous across the pair.

The parts of the boundary where a source boundary lacks a corresponding destination boundary and vice versa will get conditions from other boundary conditions under the physics interface acting as fallback boundary conditions on the nonoverlapping parts.

By default, the Wall node is used as fallback unless another feature has been selected for the boundary.

About Pairs

LOCATION IN USER INTERFACE

Right-click the physics interface and select **Pairs** > **Continuity**.

Ribbon

Physics tab with the physics interface selected:

Pairs > **Continuity**

Theory for the Single-Phase Flow Interfaces

The theory for the Single-Phase Flow, Laminar Flow interface is described in this section:

- General Single-Phase Flow Theory
- Compressible Flow
- Weakly Compressible Flow
- The Mach Number Limit
- Incompressible Flow
- The Reynolds Number
- Non-Newtonian Flow
- Gravity
- Theory for the Wall Boundary Condition
- Prescribing Inlet and Outlet Conditions
- Mass Flow
- Fully Developed Flow (Inlet)
- Fully Developed Flow (Outlet)
- No Viscous Stress
- Normal Stress Boundary Condition
- Porous Interface
- Mass Sources for Fluid Flow
- Numerical Stability — Stabilization Techniques for Fluid Flow
- Solvers for Laminar Flow
- Pseudo Time Stepping for Laminar Flow Models
- Nitsche Constraints

- Particle Tracing in Fluid Flow
- References for the Single-Phase Flow, Laminar Flow Interfaces

The theory about most boundary conditions is found in Ref. 2.

General Single-Phase Flow Theory

The Single-Phase Fluid Flow interfaces are based on the Navier–Stokes equations, which in their most general form read

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \tag{3-4}$$

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \cdot [-p\mathbf{I} + \mathbf{K}] + \mathbf{F} \tag{3-5}$$

$$\rho C_p \left(\frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla)T \right) = -(\nabla \cdot \mathbf{q}) + \mathbf{K}:\mathbf{S} - \frac{T}{\rho} \frac{\partial \rho}{\partial T}\bigg|_p \left(\frac{\partial p}{\partial t} + (\mathbf{u} \cdot \nabla)p \right) + Q \tag{3-6}$$

where

- ρ is the density (SI unit: kg/m^3)
- $\mathbf{u}$ is the velocity vector (SI unit: m/s)
- p is pressure (SI unit: Pa)
- $\mathbf{I}$ is the identity matrix (unitless)
- $\mathbf{K}$ is the viscous stress tensor (SI unit: Pa)
- $\mathbf{F}$ is the volume force vector (SI unit: N/m^3)
- C_p is the specific heat capacity at constant pressure (SI unit: J/(kg·K))
- T is the absolute temperature (SI unit: K)
- $\mathbf{q}$ is the heat flux vector (SI unit: W/m^2)
- Q contains the heat sources (SI unit: W/m^3)
- $\mathbf{S}$ is the strain-rate tensor:

$$\mathbf{S} = \frac{1}{2}(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$$

The operation ":" denotes a contraction between tensors defined by

$$\mathbf{a}:\mathbf{b} = \sum_n \sum_m a_{nm} b_{nm} \tag{3-7}$$

This is sometimes referred to as the double dot product.

Equation 3-4 is the continuity equation and represents conservation of mass. Equation 3-5 is a vector equation which represents conservation of momentum. Equation 3-6 describes the conservation of energy, formulated in terms of temperature. This is an intuitive formulation that facilitates boundary condition specifications.

To close the equation system, Equation 3-4 through Equation 3-6, constitutive relations are needed.

For a Newtonian fluid, which has a linear relationship between stress and strain, Stokes (Ref. 1) deduced the following expression:

$$\mathbf{K} = 2\mu\mathbf{S} - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I} \tag{3-8}$$

The dynamic viscosity, μ (SI unit: Pa·s), for a Newtonian fluid is allowed to depend on the thermodynamic state but not on the velocity field. All gases and many liquids can be considered Newtonian.

For an inelastic non-Newtonian fluid, the relationship between stress and strain rate is nonlinear, and an apparent viscosity is introduced instead of the dynamic viscosity. Examples of non-Newtonian fluids are honey, mud, blood, liquid metals, and most polymer solutions.

With the Microfluidics Module, you can model flows of non-Newtonian fluids using the predefined constitutive models. The following models which describe the stress-strain relationship for non-Newtonian fluids are available: Power law, Carreau, Bingham–Papanastasiou, Herschel–Bulkley–Papanastasiou and Casson–Papanastasiou.

In theory, the same equations describe both laminar and turbulent flows. In practice, however, the mesh resolution required to simulate turbulence with the Laminar Flow interface makes such an approach impractical.

	There are several books where derivations of the Navier–Stokes equations and detailed explanations of concepts such as Newtonian fluids can be found. See, for example, the classical text by Batchelor (Ref. 3) and the more recent work by Panton (Ref. 4).

Many applications describe isothermal flows for which Equation 3-6 is decoupled from Equation 3-4 and Equation 3-5.

2D AXISYMMETRIC FORMULATIONS

A 2D axisymmetric formulation of Equation 3-4 and Equation 3-5 requires $\partial/\partial\phi$ to be zero. That is, there must be no gradients in the azimuthal direction. A common additional assumption is, however, that $u_\phi = 0$. In such cases, the ϕ-equation can be removed from Equation 3-5. The resulting system of equations is both easier to converge and computationally less expensive compared to retaining the ϕ-equation. The default 2D axisymmetric formulation of Equation 3-4 and Equation 3-5 therefore assumes that

$$\partial/\partial\phi = 0$$
$$u_\phi = 0$$

Compressible Flow

The equations of motion for a single-phase fluid are the continuity equation:

$$\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\mathbf{u}) = 0 \tag{3-9}$$

and the momentum equation:

$$\rho\frac{\partial\mathbf{u}}{\partial t} + \rho\mathbf{u}\cdot\nabla\mathbf{u} = -\nabla p + \nabla\cdot\left(\mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right) + \mathbf{F} \tag{3-10}$$

These equations are applicable for incompressible as well as for compressible flow with density and viscosity variations.

Weakly Compressible Flow

The same equations as for Compressible Flow are applied for weakly compressible flow. The only difference is that the density is evaluated at the reference pressure. The density may be a function of other quantities, in particular it may be temperature dependent.

The weakly compressible flow equations are valid for incompressible as well as compressible flow with density variations independent of the pressure.

Provided that the densities dependency pressure is specified through model inputs, the density is automatically evaluated at the reference pressure level.

The Mach Number Limit

An important dimensionless number in fluid dynamics is the Mach number, Ma, defined by

$$\mathrm{Ma} = \frac{|\mathbf{u}|}{a}$$

where a is the speed of sound. A flow is formally incompressible when $\mathrm{Ma} = 0$. This is theoretically achieved by letting the speed of sound tend to infinity. The Navier–Stokes equations then have the mathematical property that pressure disturbances are instantaneously propagated throughout the entire domain. This results in a parabolic equation system.

The momentum equation, Equation 3-10, is parabolic for unsteady flow and elliptic for steady flow, whereas the continuity equation, Equation 3-9, is hyperbolic for both steady and unsteady flow. The combined system of equations is thus hybrid parabolic-hyperbolic for unsteady flow and hybrid elliptic-hyperbolic for steady flow. An exception occurs when the viscous term in Equation 3-10 becomes vanishingly small, such as at an outflow boundary, in which case the momentum equation becomes locally hyperbolic. The number of boundary conditions to apply on the boundary then depends on the number of characteristics propagating into the computational domain. For the purely hyperbolic system, the number of characteristics propagating from the boundary into the domain changes as the Mach number passes through unity. Hence, the number of boundary conditions required to obtain a numerically well-posed system must also change. The compressible formulation of the laminar and turbulent interfaces uses the same boundary conditions as the incompressible formulation, which implies that the compressible interfaces are not suitable for flows with a Mach number larger than or equal to one. Yet, the practical Mach number limit is lower than one. The main reason is that the numerical scheme (stabilization and boundary conditions) of the Laminar Flow interface does not recognize the direction and speed of pressure waves. The fully compressible Navier–Stokes equations do, for example, start to display very sharp gradients already at moderate Mach numbers. But the stabilization for the single-phase flow interface does not necessarily capture these gradients. It is impossible to give an exact limit where the low Mach number regime ends and the moderate Mach number regime begins, but a rule of thumb is that the Mach number effects start

to appear at $\mathrm{Ma} = 0.3$. For this reason, the compressible formulation is referred to as *Compressible flow (Ma< 0.3)* in COMSOL Multiphysics.

Incompressible Flow

When the temperature variations in the flow are small, a single-phase fluid can often be assumed incompressible; that is, ρ is constant or nearly constant. This is the case for all liquids under normal conditions and also for gases at low velocities. For constant ρ, Equation 3-9 reduces to

$$\rho \nabla \cdot \mathbf{u} = 0 \tag{3-11}$$

and Equation 3-10 becomes

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \cdot [-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)] + \mathbf{F} \tag{3-12}$$

Provided that the densities dependency on temperature and pressure is specified through model inputs, the density is evaluated at the reference pressure level and at the reference temperature. However, if the density is a function of other quantities such as a concentration field, or if the density is specified by a user defined expression, the user has to make sure that the density is defined as constant when the incompressible flow formulation is used.

The Reynolds Number

A fundamental characteristic in analyses of fluid flow is the Reynolds number:

$$\mathrm{Re} = \frac{\rho U L}{\mu}$$

where U denotes a velocity scale, and L denotes a representative length. The Reynolds number represents the ratio between inertial and viscous forces. At low Reynolds numbers, viscous forces dominate and tend to damp out all disturbances, which leads to laminar flow. At high Reynolds numbers, the damping in the system is very low, giving small disturbances the possibility to grow by nonlinear interactions. If the Reynolds number is high enough, the flow field eventually ends up in a chaotic state called turbulence.

Note that the Reynolds number can have different meanings depending on the length scale and velocity scale. To be able to compare two Reynolds numbers, they must be based on equivalent length and velocity scales.

The Fluid Flow interfaces automatically calculate the local cell Reynolds number $\mathrm{Re}^c = \rho|\mathbf{u}|h/(2\mu)$ using the element length h for L and the magnitude of the velocity vector u for the velocity scale U. This Reynolds number is not related to the character of the flow field, but to the stability of the numerical discretization. The risk for numerical oscillations in the solution increases as Re^c grows. The cell Reynolds number is a predefined quantity available for visualization and evaluation (typically it is available as: `spf.cellRe`).

Non-Newtonian Flow

For an inelastic non-Newtonian fluid, the relationship between stress and strain rate is nonlinear, and we may express the constitutive relation in terms of an apparent viscosity. For the incompressible flow, it is:

$$\mathbf{K} = 2\mu_{\mathrm{app}}(\dot{\gamma})\ \mathbf{S}$$

where $\dot{\gamma}$ is the shear rate,

$$\dot{\gamma} = \sqrt{2\mathbf{S}:\mathbf{S}}$$

and the contraction operator ":" is defined by

$$\mathbf{a}:\mathbf{b} = \sum_n \sum_m a_{nm} b_{nm}$$

The Laminar Flow interfaces provide various predefined inelastic non-Newtonian constitutive models including Power law, Carreau, Bingham–Papanastasiou, Herschel–Bulkley–Papanastasiou and Casson–Papanastasiou.

POWER LAW

The Power law model is an example of a generalized Newtonian model. It prescribes

$$\mu_{\mathrm{app}} = m\left(\frac{\dot{\gamma}}{\dot{\gamma}_{\mathrm{ref}}}\right)^{n-1} \tag{3-13}$$

where m, n are scalars that can be set to arbitrary values and $\dot{\gamma}_{\mathrm{ref}}$ denotes a reference shear rate for which the default value is $1\ \mathrm{s}^{-1}$. For $n > 1$, the power law describes a shear thickening (dilatant) fluid. For $n < 1$, it describes a shear thinning (pseudoplastic) fluid. A value of n equal to one gives the expression for a *Newtonian fluid*.

Equation 3-13 predicts an infinite viscosity at zero shear rate for $n < 1$. This is however never the case physically. Instead, most fluids have a constant viscosity for shear rates smaller than $10^{-2}\ \mathrm{s}^{-1}$ (Ref. 18). Since infinite viscosity also makes models using Equation 3-13 difficult to solve, COMSOL Multiphysics implements the Power law model as

$$\mu_{\mathrm{app}} = m\left(\frac{\max(\dot{\gamma}, \dot{\gamma}_{\mathrm{min}})}{\dot{\gamma}_{\mathrm{ref}}}\right)^{n-1} \tag{3-14}$$

where $\dot{\gamma}_{\mathrm{min}}$ is a lower limit for the evaluation of the shear rate magnitude. The default value for $\dot{\gamma}_{\mathrm{min}}$ is $10^{-2}\ \mathrm{s}^{-1}$, but can be given an arbitrary value or expression using the corresponding text field.

CARREAU MODEL

The Carreau model defines the viscosity in terms of the following four-parameter expression

$$\mu_{\mathrm{app}} = \mu_\infty + (\mu_0 - \mu_\infty)[1 + (\lambda\dot{\gamma})^2]^{\frac{n-1}{2}} \tag{3-15}$$

where λ is a parameter with the unit of time, μ_0 is the zero shear rate viscosity, μ_∞ is the infinite shear-rate viscosity, and n is a dimensionless parameter. This expression is able to describe the viscosity for most stationary polymer flows.

BINGHAM–PAPANASTASIOU

Viscoplastic fluid behavior is characterized by existence of the yield stress τ_y — a limit which must be exceeded before significant deformation can occur. To model the stress-deformation behavior of viscoplastic materials, different constitutive equations have been propose. The Bingham plastic model is written as

$$\mu_{\mathrm{app}} = \mu_p + \frac{\tau_y}{\dot{\gamma}}, \quad |\mathbf{K}| > \tau_y$$

where μ_p is the plastic viscosity.

To allow computation in both yielded and unyielded region, the Papanastasiou continuous regularization for the viscosity function is used:

$$\mu_{\mathrm{app}} = \mu_p + \frac{\tau_y}{\dot{\gamma}}[1 - \exp(-m_p\dot{\gamma})] \tag{3-16}$$

where m_p is a scale that controls the exponential growth of stress.

HERSCHEL–BULKLEY–PAPANASTASIOU

The Herschel–Bulkley –Papanastasiou model combines the effects of the Power law the Papanastasiou continuous regularization:

$$\mu_{app} = m\left(\frac{\dot{\gamma}}{\dot{\gamma}_{ref}}\right)^{n-1} + \frac{\tau_y}{\dot{\gamma}}[1 - \exp(-m_p\dot{\gamma})] \tag{3-17}$$

where m, n are scalars that can be set to arbitrary values, and $\dot{\gamma}_{ref}$ is the reference shear rate. In case n equals one, the Bingham–Papanastasiou model is recovered. This equation is valid in both yielded and unyielded regions. The exponent m_p controls the smoothness of the viscosity function.

CASSON–PAPANASTASIOU

The Casson–Papanastasiou model combines Casson equation with the Papanastasiou regularization:

$$\mu_{app} = \left(\sqrt{\mu_p} + \sqrt{\frac{\tau_y}{\dot{\gamma}}}[1 - \exp(-\sqrt{m_p\dot{\gamma}})]\right)^2 \tag{3-18}$$

The equation is valid in both yielded and unyielded regions.

Gravity

DEFINITION

The gravity force is defined from the acceleration of gravity vector, $\mathbf{g}$, and the density, ρ. Under usual conditions and in Cartesian coordinates with the z-axis in the vertical direction,

$$\mathbf{g} = \begin{pmatrix} 0 \\ 0 \\ -g_{const} \end{pmatrix}.$$

When gravity is considered, a volume force equal to $\rho\mathbf{g}$ is included in the momentum equation. For example, for laminar weakly compressible flow, it reads:

$$\rho\frac{\partial \mathbf{u}}{\partial t} + \rho\mathbf{u}\cdot\nabla\mathbf{u} = \nabla\cdot\left(-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right) + \mathbf{F} + \rho\mathbf{g} \qquad (3\text{-}19)$$

Introducing a constant reference density ρ_{ref}, and assuming that $\mathbf{g}$ is homogeneous, this equation is equivalently written:

$$\begin{aligned}&\rho\frac{\partial \mathbf{u}}{\partial t} + \rho\mathbf{u}\cdot\nabla\mathbf{u} = \\ &\nabla\cdot\left(-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I} + \rho_{\text{ref}}\mathbf{g}\cdot(\mathbf{r}-\mathbf{r}_{\text{ref}})\right) + \mathbf{F} + (\rho-\rho_{\text{ref}})\mathbf{g}\end{aligned} \qquad (3\text{-}20)$$

where $\mathbf{r}$ is the position vector and $\mathbf{r}_{\text{ref}}$ is an arbitrary reference position vector.

From this equation, it is convenient to define the reduced pressure which accounts for the hydrostatic pressure, $\tilde{p} = p - \rho_{\text{ref}}\mathbf{g}\cdot(\mathbf{r}-\mathbf{r}_{\text{ref}})$

$$\begin{aligned}&\rho\frac{\partial \mathbf{u}}{\partial t} + \rho\mathbf{u}\cdot\nabla\mathbf{u} = \nabla\cdot\left(-\tilde{p}\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right) + \\ &\mathbf{F} + (\rho-\rho_{\text{ref}})\mathbf{g}\end{aligned} \qquad (3\text{-}21)$$

In Equation 3-21, the gravity force is written $(\rho-\rho_{\text{ref}})\mathbf{g}$.

PRESSURE FORMULATION

When the relative pressure is used (default option) the interface dependent variable represents the relative pressure and the absolute pressure is defined as $p_A = p_{\text{ref}} + p$. When the pressure is used to define a boundary condition (for example, when p_0 defines the pressure condition at an outlet), it represents the relative pressure. Hence defining the outlet pressure as $p_{\text{hydro,approx}} = -\rho_{\text{ref}}\mathbf{g}\cdot(\mathbf{r}-\mathbf{r}_{\text{ref}})$ compensates for the gravity force for an ambient reference pressure of 0 Pa when the density is constant, there is no external force, and provided p_{ref}, $\mathbf{g}$, and $\mathbf{r}_0$ are defined consistently.

When the reduced pressure is used, the interface dependent variable (named p by default) represents the reduced pressure. The absolute pressure is then defined as $p_A = p_{\text{ref}} - \rho_{\text{ref}}\mathbf{g}\cdot(\mathbf{r}-\mathbf{r}_{\text{ref}}) + p$. In this case when the pressure is used to define a boundary condition (for example, to define a pressure condition at an outlet), its value corresponds to the reduced pressure. Hence, the prescribed pressure compensates for an approximate hydrostatic pressure, $p_{\text{hydro,approx}} = -\rho_{\text{ref}}\mathbf{g}\cdot(\mathbf{r}-\mathbf{r}_{\text{ref}})$, which is exact only when the density is constant and there is no external force.

PRESSURE BOUNDARY CONDITION

For an immobile fluid the momentum equation simplifies to $\nabla \cdot (p\mathbf{I}) = \mathbf{F} + \rho\mathbf{g}$ or

$\nabla \cdot (-\tilde{p}\mathbf{I}) = \mathbf{F} + (\rho - \rho_{ref})\mathbf{g}$ depending on the pressure formulation.

For incompressible flow, assuming there are no external forces, this leads respectively to $p = -\rho_{ref}\mathbf{g} \cdot (\mathbf{r} - \mathbf{r}_{ref}) + p_0$ or $\tilde{p} = p_0$.

Theory for the Wall Boundary Condition

See Wall for the node settings.

SLIP

The Slip condition assumes that there are no viscous effects at the slip wall and hence, no boundary layer develops. From a modeling point of view, this is a reasonable approximation if the important effect of the wall is to prevent fluid from leaving the domain. Mathematically, the constraint can be formulated as:

$$\mathbf{u} \cdot \mathbf{n} = 0, \qquad (-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^{\mathrm{T}}))\mathbf{n} = \mathbf{0}$$

The no-penetration term takes precedence over the Neumann part of the condition and the above expression is therefore equivalent to

$$\mathbf{u} \cdot \mathbf{n} = 0, \qquad \mathbf{K}_n - (\mathbf{K}_n \cdot \mathbf{n})\mathbf{n} = \mathbf{0}$$
$$\mathbf{K}_n = \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^{\mathrm{T}})\mathbf{n}$$

expressing that there is no flow across the boundary and no viscous stress in the tangential direction.

For a moving wall with translational velocity $\mathbf{u}_{tr}$, $\mathbf{u}$ in the above equations is replaced by the relative velocity $\mathbf{u}_{rel} = \mathbf{u} - \mathbf{u}_{tr}$.

The boundary condition for ν is $\nabla\nu \cdot \mathbf{n} = 0$.

POROUS SLIP

The **Porous slip** option, which can be chosen in the **Porous treatment of no slip condition** list when **Enable porous media domains** is activated, results in a special treatment of **Wall** boundaries and **Interior Wall** boundaries adjacent to porous domains (**Porous Medium** feature). Namely, similar to the **Navier slip** boundary condition, no penetration and tangential stress conditions are applied at the wall:

$$\mathbf{u}\cdot\mathbf{n} = 0, \qquad \mathbf{K}_n - (\mathbf{K}_n\cdot\mathbf{n})\mathbf{n} = -\frac{\mu}{\varepsilon_p}\frac{\mathbf{u}_{slip}}{y_{ps}},$$

$$\mathbf{u}_{slip} = \mathbf{u} - (\mathbf{u}\cdot\mathbf{n})\mathbf{n}, \qquad \mathbf{K}_n = \frac{\mu}{\varepsilon_p}(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)\mathbf{n}$$

Here, $\mathbf{K}_n$ is the viscous wall traction, $\mathbf{n}$ is the wall normal, $\mathbf{u}_{slip}$ is the tangential velocity at the wall while real no slip is assumed to be applied at a distance d_w (half-height of the first cell adjacent to the wall) outside the wall, and ν_{ps} is the porous slip length. An analytical derivation of the velocity profile in the boundary layer where the pressure gradient is balanced by the sum of the Darcy term, the Forchheimer drag, and the viscous term (neglecting convective terms) leads to the following expression for y_{ps}:

$$y_{ps} = \tilde{l}\left(\frac{1+X_p e^{-\xi_p}}{1-X_p e^{-\xi_p}}\right)\left[\left(\frac{1+X_p e^{-\xi_p}}{1+X_p}\right)^2 e^{\xi_p} - 1\right], \quad \xi_p = \frac{d_w}{\tilde{l}}, \quad \tilde{l} = \frac{l_{pore}}{\sqrt{1+2c_\beta}},$$

$$X_p = \frac{\sqrt{1+2c_\beta} - \sqrt{1+\frac{4}{3}c_\beta}}{\sqrt{1+2c_\beta} + \sqrt{1+\frac{4}{3}c_\beta}}, \qquad c_\beta = \frac{\sqrt{1+4c_D}-1}{2}, \; c_D = \frac{\beta_{ND}}{\mu}\frac{\kappa^2}{\mu}|\nabla p - \rho\mathbf{g}|$$

where $l_{pore} = \sqrt{\kappa/\varepsilon_p}$ is the porous length scale, $\beta_{ND} = \rho c_F/\sqrt{\kappa}$ is the non-Darcian coefficient (c_F is the Forchheimer coefficient), $\mathbf{g}$ is the gravity vector, and ξ_p, l, X_p, c_β, c_D, are intermediate variables. This formula is used when the **Pressure-gradient formulation** is chosen and it uses the pressure gradient at the wall. By default, the **Velocity formulation** is activated and the corresponding formula is:

$$y_{ps} = \tilde{l}\,(e^{\xi_p} - 1), \quad \xi_p = \frac{d_w}{\tilde{l}}, \quad \tilde{l} = \frac{l_{pore}}{\sqrt{1+2c_\beta}},$$

$$c_\beta = \left[\left(\frac{\beta_{ND}\kappa|\mathbf{u}_{slip}|}{\mu}\frac{l_{pore}}{d_w}\right)^2/2\right]^{1/3}$$

Although this formulation is an approximation, since it uses the slip velocity at the wall to reconstruct the pressure gradient, it is rather accurate. Moreover, the influence of the convective terms is partially accounted for in this formulation.

SLIDING WALL

The sliding wall option is appropriate if the wall behaves like a conveyor belt; that is, the surface is sliding in its tangential direction. The wall does not have to actually move in the coordinate system.

- In 2D, the tangential direction is unambiguously defined by the direction of the boundary, but the situation becomes more complicated in 3D. For this reason, this boundary condition has slightly different definitions in the different space dimensions.
- For 2D and 2D axisymmetric components, the velocity is given as a scalar U_w and the condition prescribes

$$\mathbf{u} \cdot \mathbf{n} = 0, \qquad \mathbf{u} \cdot \mathbf{t} = U_w$$

  where $\mathbf{t} = (n_y, -n_x)$ for 2D and $\mathbf{t} = (n_z, -n_r)$ for axial symmetry.
- For 3D components, the velocity is set equal to a given vector $\mathbf{u}_w$ projected onto the boundary plane:

$$\mathbf{u} = \frac{\mathbf{u}_w - (\mathbf{n} \cdot \mathbf{u}_w)\mathbf{n}}{\|\mathbf{u}_w - (\mathbf{n} \cdot \mathbf{u}_w)\mathbf{n}\|}\|\mathbf{u}_w\|$$

  The normalization makes $\mathbf{u}$ have the same magnitude as $\mathbf{u}_w$ even if $\mathbf{u}_w$ is not exactly parallel to the wall.

SLIP VELOCITY

In the microscale range, the flow at a boundary is seldom strictly no slip or slip. Instead, the boundary condition is something in between, and there is a slip velocity at the boundary. Two phenomena account for this velocity: violation of the continuum hypothesis for the viscosity and flow induced by a thermal gradient along the boundary.

The following equation relates the viscosity-induced jump in tangential velocity to the tangential shear stress along the boundary:

$$\Delta u = \frac{1}{\beta}\tau_{n,t}$$

For gaseous fluids, the coefficient β is given by

$$\beta = \frac{\mu}{\left(\frac{2-\alpha_v}{\alpha_v}\right)\lambda}$$

where μ is the fluid's dynamic viscosity (SI unit: Pa·s), α_v represents the tangential momentum accommodation coefficient (TMAC) (dimensionless), and λ is the molecules' mean free path (SI unit: m). The tangential accommodation coefficients are typically in the range of 0.85 to 1.0 and can be found in Ref. 17.

A simpler expression for β is

$$\beta = \frac{\mu}{L_s}$$

where L_s, the slip length (SI unit: m), is a straight channel measure of the distance from the boundary to the virtual point outside the flow domain where the flow profile extrapolates to zero. This equation holds for both liquids and gases.

Thermal creep results from a temperature gradient along the boundary. The following equation relates the thermally-induced jump in tangential velocity to the tangential gradient of the natural logarithm of the temperature along the boundary:

$$\Delta u = \sigma_T \frac{\mu}{\rho} \nabla_t \log T$$

where σ_T is the thermal slip coefficient (dimensionless) and ρ is the density of the fluid. The thermal slip coefficients range between 0.3 and 1.0 and can be found in Ref. 17.

Combining the previous relationships results in the following equation:

$$\mathbf{u} - \mathbf{u}_{w,t} = \frac{L_s}{\mu} \tau_{n,t} + \sigma_T \frac{\mu}{\rho T} \nabla_t T$$

Relate the tangential shear stress to the viscous boundary force by

$$\tau_{n,t} = \mathbf{K}_n - (\mathbf{n} \cdot \mathbf{K}_n)\mathbf{n}$$

where the components of $\mathbf{K}$ are the Lagrange multipliers that are used to implement the boundary condition. Similarly, the tangential temperature gradient results from the difference of the gradient and its normal projection:

$$\nabla_t T = \nabla T - (\mathbf{n} \cdot \nabla T)\mathbf{n}$$

Use Viscous Slip

When viscous slip is used, select Maxwell's model to calculate L_s using:

$$L_s = \left(\frac{2 - \alpha_v}{\alpha_v}\right)\lambda$$

Also see Wall for the node settings.

ELECTROOSMOTIC VELOCITY

Most solid surfaces acquire a surface charge when brought into contact with an electrolyte. In response to the spontaneously formed surface charge, a charged solution forms close to the liquid-solid interface. This is known as an electric double layer. If an electric field is applied to the fluid, this very narrow layer starts to move along the boundary.

It is possible to model the fluid's velocity near the boundary using the Helmholtz–Smoluchowski relationship between the electroosmotic velocity u and the applied electric field:

$$u = \mu_{eo}\mathbf{E}_t$$

where μ_{eo} is the electroosmotic mobility and $\mathbf{E}_t$ is the fluid electric field tangential to the wall.

Built-in Expression

Use the Electroosmotic mobility μ_{eo} (SI unit: $m^2/(s\cdot V)$) Built-in expression to compute the electroosmotic mobility from:

$$\mu_{eo} = -\varepsilon_r\varepsilon_0\frac{\zeta}{\mu} \tag{3-22}$$

Here ε_r is the fluid's relative permittivity, ε_0 the permittivity of free space (SI unit F/m), which is a predefined physical constant, ζ is the fluid's zeta potential (SI unit: V), and μ the fluid's dynamic viscosity (Pa·s). Typically $\mu_{eo} \approx 7 \times 10^{-8}\ m^2/(s\cdot V)$ and $\zeta \approx 100$ mV (see H. Bruus, *Theoretical Microfluidics*, Oxford University Press, 2008). See Wall for the node settings.

	Electroosmotic Micromixer: Application Library path **Microfluidics_Module/Micromixers/electroosmotic_mixer**

Navier Slip

This boundary condition enforces no-penetration at the wall, $\mathbf{u} \cdot \mathbf{n}_{wall} = 0$, and adds a tangential stress

$$\mathbf{K}_{nt} = -\frac{\mu}{\beta}\mathbf{u}_{slip}$$

where $\mathbf{K}_{nt} = \mathbf{K}_n - (\mathbf{K}_n \cdot \mathbf{n}_{wall})\mathbf{n}_{wall}$, $\mathbf{K}_n = \mathbf{K}\mathbf{n}_{wall}$, and $\mathbf{K}$ is the viscous stress tensor. β is a slip length, and $\mathbf{u}_{slip} = \mathbf{u} - (\mathbf{u} \cdot \mathbf{n}_{wall})\mathbf{n}_{wall}$ is the velocity tangential to the wall. The boundary condition does not set the tangential velocity component to zero; however, the extrapolated tangential velocity component is 0 at a distance β outside the wall.

The **Slip Length** setting is per default set to **Factor of minimum element length**. The slip length β is then defined as $\beta = f_h h_{min}$, where h_{min} is the smallest element side (corresponds to the element size in the wall normal direction for boundary layer elements) and f_h is a user input.

In cases where the wall movement is nonzero, **Account for the translational wall velocity in the friction force** may be selected to use $\mathbf{u} - \mathbf{u}_{bnd} - ((\mathbf{u} - \mathbf{u}_{bnd}) \cdot \mathbf{n}_{wall})\mathbf{n}_{wall}$ instead of $\mathbf{u}_{slip}$ in the friction force. Then, the extrapolated tangential velocity component is $\mathbf{u}_{bnd}$ at a distance β outside of the wall. Note that the **Velocity of sliding wall** $\mathbf{u}_w$ is always accounted for in the friction force.

The Navier Slip boundary condition is suitable for walls adjacent to a fluid-fluid interface or a free surface when solving for laminar flow. Applying this boundary condition, the contact line (fluid-fluid-solid interface) is free to move along the wall. Note that in problems with contact lines, the tangential velocity of the wall typically represents the movement of the contact line but the physical wall is not moving. In such cases, **Account for the translational wall velocity in the friction force** should not be checked.

The Navier Slip option is not available when selecting a turbulence model.

CONSTRAINT SETTINGS

The wall feature uses three different techniques to constrain the velocity field:

- **Pointwise constraints** is the standard technique to enforce strong constraints in the finite element method. The desired value of the velocity is prescribed at each node point in the mesh. Since the constraint is enforced locally at each node, only local values are affected by the constraint and the constraints are independent of each other. The solvers can therefore eliminate both the constrained degrees of freedom and the constraint force terms, effectively reducing the number of degrees of freedom being solved for.

  The main advantage of pointwise constraints is that they enforce the constraint exactly pointwise. This means that they do not introduce any leakage of the velocity across the wall, unless specified. The main disadvantage of pointwise constraints is that they introduce locking effects when trying to impose a no-penetration condition for the velocity, $\mathbf{u} \cdot \mathbf{n} = 0$, on curved walls or walls with sharp corners.

- **Weak constraints** is an alternative method to prescribe the velocity. It consists on enforcing the boundary condition for the velocity via *Lagrange multipliers*. Their main advantage is that the Lagrange multiplier can provide an accurate representation of the reaction flux at the wall. Their main disadvantage is that they introduce extra unknowns, and are usually difficult to combine with other constraint methods on adjacent boundaries. Moreover, they may require extra constraints for the Lagrange multipliers. For more information, see Weak Constraints in the *COMSOL Multiphysics Reference Manual*.
- **Nitsche constraints** use a numerical flux to prescribe the velocity at the wall. They impose the constraint in an integral sense rather than pointwise, and do not suffer from the locking effects introduced by pointwise constraints when trying to prescribe a no penetration condition for the velocity. They are also better behaved when prescribing nonlinear constraints. Their main disadvantage is that the constraint is only imposed approximately, and may produce small leaks. For more information, see Nitsche Constraints.

The following combination of Constraint techniques can be selected in the **Constraint Setting** sections of Wall boundary conditions:

- **Automatic** (default) use different constraint methods depending on whether only the normal component of the velocity is prescribed, such as in the no penetration condition, $\mathbf{u} \cdot \mathbf{n} = 0$, imposed, for example, in Slip walls or No Slip walls using Wall Functions or Automatic Wall Treatment, or both tangential and normal components are prescribed, as is the case of No Slip walls in laminar flow.

  Nitsche constraints are used to impose the no penetration condition for Slip walls. When a No Slip condition is prescribed, pointwise constraints are used except for moving walls where Nitsche constraints are used.
- **Pointwise constraints**
- **Nitsche constraints**
- **Weak constraints** — these are not available on Interior Walls.
- **Mixed constraints** — this option is only available when both the tangential and normal components of the velocity need to be prescribed. The velocity on the wall normal direction is imposed via pointwise constraints. The constraint for the tangential directions is relaxed, and Nitsche constraints are used instead. This provides improved accuracy and performance when working with coarse boundary layer meshes. For more information, see Ref. 19.

Prescribing Inlet and Outlet Conditions

The Navier–Stokes equations can show large variations in mathematical behavior, ranging from almost completely elliptic to almost completely hyperbolic. This has implications when it comes to prescribing admissible boundary conditions. There is also a discrepancy between mathematically valid boundary conditions and practically useful boundary conditions. See Inlet and Outlet for the node settings.

INLET CONDITIONS

An inlet requires specification of the velocity components. The most robust way to do this is to prescribe a velocity field using a Velocity condition.

A common alternative to prescribing the complete velocity field is to prescribe a pressure and all but one velocity component. The pressure cannot be specified pointwise because this is mathematically over-constraining. Instead the pressure can be specified via a stress condition:

$$-p + 2\mu\frac{\partial u_n}{\partial n} = F_n \tag{3-23}$$

where $\partial u_n/\partial n$ is the normal derivative of the normal velocity component. Equation 3-23 is prescribed by the Pressure condition in the Inlet and Outlet features and the Normal stress condition in the Open Boundary and Boundary Stress features. Equation 3-23 is mathematically more stringent compared to specifying the pressure pointwise and at the same time cannot guarantee that p obtains the desired value. In practice, p is close to F_n, except for low Reynolds number flows where viscous effects are the only effects that balance the pressure. In addition to Equation 3-23, all but one velocity component must be specified. For low Reynolds numbers, this can be specified by a vanishing tangential stress condition:

$$\mu\frac{\partial u_t}{\partial n} = 0$$

which is what the Normal stress condition does. Vanishing tangential stress becomes a less well-posed inlet condition as the Reynolds number increases. The Pressure condition in the Inlet feature therefore requires a flow direction to be prescribed, which provides a well-posed condition independent of Reynolds number.

OUTLET CONDITIONS

The most common approach is to prescribe a pressure via a normal stress condition on the outlet. This is often accompanied by a vanishing tangential stress condition:

$$\mu \frac{\partial u_t}{\partial n} = 0$$

where $\partial u_t/\partial n$ is the normal derivative of the tangential velocity field. It is also possible to prescribe u_t to be zero. The latter option should be used with care since it can have a significant effect on the upstream solution.

The elliptic character of the Navier–Stokes equations mathematically permits specifying a complete velocity field at an outlet. This can, however, be difficult to apply in practice. The reason being that it is hard to prescribe the outlet velocity so that it is consistent with the interior solution at each point. The adjustment to the specified velocity then occurs across an outlet boundary layer. The thickness of this boundary layer depends on the Reynolds number; the higher the Reynolds number, the thinner the boundary layer.

ALTERNATIVE FORMULATIONS

COMSOL Multiphysics provides several specialized boundary conditions that either provide detailed control over the flow at the boundary or that simulate specific devices. In practice they often prescribe a velocity or a pressure but calculate the prescribed values using, for example, ODEs.

Normal Stress Boundary Condition

Mass Flow

The **Mass flow** boundary condition constrains the mass flowing into the domain across an inlet or outlet boundary. The mass flow can be specified in a number of ways.

POINTWISE MASS FLUX

The pointwise mass flux sets the velocity at the boundary to

$$\mathbf{u} = -\frac{m_f}{\rho}\mathbf{n}$$

where m_f is the normal mass flux and ρ is the density.

MASS FLOW RATE

The mass flow rate boundary condition sets the total mass flow through the inlet boundary according to

$$-\int_{\partial\Omega} d_{bc}\rho(\mathbf{u}\cdot\mathbf{n})\mathrm{d}S = m$$

where d_{bc} (only present in the 2D Cartesian axis system) is the boundary thickness normal to the fluid-flow domain and m is the total mass flow rate. For the outlet boundary, the mass flow rate boundary condition sets the total mass flow as

$$\int_{\partial\Omega} d_{bc}\rho(\mathbf{u}\cdot\mathbf{n})\mathrm{d}S = m$$

In addition to the constraint on the total flow across the boundary, the tangential velocity components are set to zero on the boundary

$$\mathbf{u}\times\mathbf{n} = \mathbf{0} \tag{3-24}$$

STANDARD FLOW RATE

The standard flow rate boundary condition specifies the mass flow as a standard volumetric flow rate. The mass flow through the inlet boundary is set by the equation

$$-\int_{\partial\Omega} d_{\mathrm{bc}}\frac{\rho}{\rho_{\mathrm{st}}}(\mathbf{u}\cdot\mathbf{n})\mathrm{d}S = Q_{\mathrm{sv}}$$

where d_{bc} (only present in the 2D component Cartesian axis system) is the boundary thickness normal to the fluid-flow domain, ρ_{st} is the standard density, and Q_{sv} is the standard flow rate. The standard density is defined by one of the following equations:

$$\rho_{\mathrm{st}} = \frac{M_n}{V_n}$$

$$\rho_{\mathrm{st}} = \frac{p_{\mathrm{st}}M_n}{RT_{\mathrm{st}}}$$

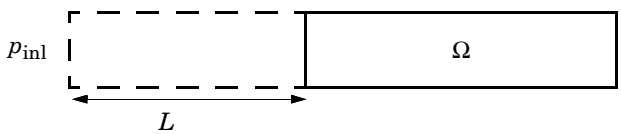
where M_n is the mean molar mass of the fluid, V_n is the standard molar volume, p_{st} is the standard pressure, R is the universal molar gas constant, and T_{st} is the standard temperature. For the outlet boundary, the mass flow rate is set by the equation

$$\int_{\partial\Omega} d_{\mathrm{bc}} \frac{\rho}{\rho_{\mathrm{st}}} (\mathbf{u} \cdot \mathbf{n}) \mathrm{d}S = Q_{\mathrm{sv}}$$

Equation 3-24 or Equation 3-25 is also enforced for compressible and incompressible flow, respectively, ensuring that the normal component of the viscous stress and the tangential component of the velocity are zero at the boundary.

Fully Developed Flow (Inlet)

The **Fully developed flow** boundary condition can be understood from the following figure:



The flow to the domain Ω is assumed to enter through a straight channel of length L. The channel is a virtual extrusion of the inlet cross section and a pressure constant pressure P_{inl} is applied on the inlet of the virtual channel.

The Fully Developed Flow boundary condition prescribes that the tangential flow component on the boundary is zero:

$$\mathbf{u} - (\mathbf{u} \cdot \mathbf{n})\mathbf{n} = \mathbf{0}$$

The momentum equation for a fully developed flow in the virtual extrusion of the inlet cross section can then be projected onto the inlet boundary with the following weak equation as the result:

$$\int_{\partial\Omega} \left(\left(L \left(-\mu (\nabla_{\mathbf{t}} \mathbf{u} + (\nabla_{\mathbf{t}} \mathbf{u})^T) + \frac{(p + P_{\mathrm{inl}})}{2} \mathbf{I} \right) : (\nabla_{\mathbf{t}} \hat{\mathbf{u}}) \right) - P_{\mathrm{inl}} (\mathbf{n} \cdot \hat{\mathbf{u}}) \right)$$

The exact value of L is somewhat arbitrary as long as it is not too high or too low. L is therefore set to ten times the inlet edge length in 2D and to ten times the square root of the inlet area in 2D axisymmetry and in 3D.

The fact that the velocity profile is not prescribed, but rather the solution of a projected weak contribution, means that the actual velocity profile that is obtained on the inlet can deviate from the analytical fully developed flow profile (in cases such an analytical solution exists) if required by the solution inside the computational domain, Ω. This is

most notably if the flow is strongly curved just downstream of the inlet. This can, for example, be the case if an object is positioned just downstream of the inlet or if the adjacent boundaries are not orthogonal to the inlet. The analytical solution can in these cases be recovered by including a little bit of the inlet channel in the computational domain.

The inlet pressure, P_{inl}, must be solved for and the its equation is a discrete algebraic equation (DAE) for P_{inl}. When, for example, the average velocity is specified, the DAE reads

$$(\langle \mathbf{u} \cdot \mathbf{n} \rangle + U_{\text{av}})\hat{P}_{\text{inl}}$$

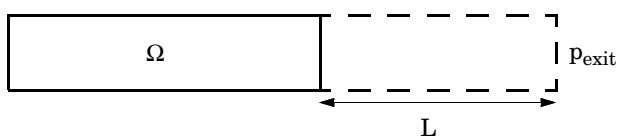
where <·> denotes the average over the inlet. Since the equation for P_{inl} is a DAE (the equation for P_{inl} does not contain P_{inl}), it must be solved coupled to Navier–Stokes and it must be treated by a Vanka presmoother and postsmoother if iterative solvers are used.

The boundary conditions for the virtual inlet channel are inherited from the boundaries adjacent to the inlet channel. Virtual boundaries adjacent to walls (except slip walls) are treated as no-slip walls. Virtual boundaries adjacent to any other type of boundary are treated as slip-walls (or equivalently as symmetry boundaries). So in the figure above, if the lower boundary of Ω is a no-slip wall and the top boundary is a symmetry boundary, the lower boundary of the virtually extruded channel becomes a no-slip wall and the upper boundary becomes a symmetry boundary.

Algebraic turbulence models need additional equations or constraints. For all other turbulence models, their weak equations in the virtual inlet channel are projected onto the inlet of the computational domain. The projections are regularized to prevent the production to fall to zero, so the solutions of the projects can show slight deviation from the correct solutions close to no-slip walls.

Fully Developed Flow (Outlet)

The **Fully developed flow** boundary condition can be understood from the following figure:



The flow to the domain Ω is assumed to enter through a straight channel of length L. The channel is a virtual extrusion of the inlet cross section and a pressure constant pressure P_{exit} is applied on the inlet of the virtual channel.

The Fully Developed Flow boundary condition prescribes that the tangential flow component on the boundary is zero:

$$\mathbf{u} - (\mathbf{u} \cdot \mathbf{n})\mathbf{n} = \mathbf{0}$$

The momentum equation for a fully developed flow in the virtual extrusion of the inlet cross section can then be projected onto the inlet boundary with the following weak equation as the result:

$$\int_{\partial\Omega} \left(\left(L \left(-\mu(\nabla_{\mathbf{t}}\mathbf{u} + (\nabla_{\mathbf{t}}\mathbf{u})^T) + \frac{(p + P_{\text{exit}})}{2}\mathbf{I} \right) : (\nabla_{\mathbf{t}}\hat{\mathbf{u}}) \right) - P_{\text{exit}}(\mathbf{n} \cdot \hat{\mathbf{u}}) \right)$$

The exact value of L is somewhat arbitrary as long as it is not too high or too low. L is therefore set to ten times the inlet edge length in 2D and to ten times the square root of the inlet area in 2D axisymmetry and in 3D.

The fact that the velocity profile is not prescribed, but rather the solution of a projected weak contribution, means that the actual velocity profile that is obtained on the outlet can deviate from the analytical fully developed flow profile (in cases such an analytical solution exists) if required by the solution inside the computational domain, Ω. The inlet pressure, P_{exit}, must be solved for and the its equation is a discrete algebraic equation (DAE) for P_{exit}. When, for example, the average velocity is specified, the DAE reads

$$(\langle \mathbf{u} \cdot \mathbf{n} \rangle + U_{\text{av}})\hat{P}_{\text{exit}}$$

where <·> denotes the average over the inlet. Since the equation for P_{ext} is a DAE, it must be solved coupled to Navier–Stokes and it must be treated by a Vanka presmoother and postsmoother if iterative solvers are used.

The boundary conditions for the virtual outlet channel are inherited from the boundaries adjacent to the outlet channel. Virtual boundaries adjacent to walls (except slip walls) are treated as no-slip walls. Virtual boundaries adjacent to any other type of boundary are treated as slip-walls (or equivalently as symmetry boundaries).

No Viscous Stress

For this module, and in addition to the Pressure, No Viscous Stress boundary condition, the viscous stress condition sets the viscous stress to zero:

$$\left(\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)-\frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right)\mathbf{n} = \mathbf{0}$$

$$(\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T))\mathbf{n} = \mathbf{0}$$

using the compressible/weakly compressible and the incompressible formulation, respectively.

The condition is not a sufficient outlet condition since it lacks information about the outlet pressure. It must hence be combined with pressure point constraints on one or several points or lines surrounding the outlet.

This boundary condition is numerically the least stable outlet condition, but can still be beneficial if the outlet pressure is nonconstant due to, for example, a nonlinear volume force.

Normal Stress Boundary Condition

The total stress on the boundary is set equal to a stress vector of magnitude f_0, oriented in the negative normal direction:

$$\left(-p\mathbf{I}+\left(\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)-\frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right)\right)\mathbf{n} = -f_0\mathbf{n}$$

$$(-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T))\mathbf{n} = -f_0\mathbf{n}$$

using the compressible/weakly compressible and the incompressible formulation, respectively.

This implies that the total stress in the tangential direction is zero. This boundary condition implicitly sets a constraint on the pressure which for 2D flows is

$$p = 2\mu\frac{\partial u_n}{\partial n}+f_0 \tag{3-25}$$

If $\partial u_n/\partial n$ is small, Equation 3-25 states that $p \approx f_0$.

The Normal Stress condition is the mathematically correct version of the Pressure Conditions condition (Ref. 4), but it is numerically less stable.

Pressure Boundary Condition

For single-phase flow, a mathematically correct natural boundary condition for outlets is

$$\left(-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)-\frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right)\mathbf{n} = -p_0\mathbf{n} \tag{3-26}$$

$$(-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T))\mathbf{n} = -p_0\mathbf{n} \tag{3-27}$$

using the compressible/weakly compressible and the incompressible formulation, respectively.

This is a normal stress condition together with a no-tangential-stress condition. When $\mu > 0$, Equation 3-26 or Equation 3-27 can be supplemented with a tangential velocity condition

$$\mathbf{u}\cdot\mathbf{t} = 0 \tag{3-28}$$

If so, the no-tangential-stress condition is overridden. An issue with Equation 3-26 or Equation 3-27 is that it does not strongly enforce unidirectional flow on the boundary. If the prescribed pressure on an outlet is too high, parts of the outlet can actually have inflow. This is not as much of an issue for the Navier–Stokes equations as it is an issue for scalar transport equations solved along with the Navier–Stokes equations. Hence, when applying the **Pressure** boundary condition at an outlet or inlet you can further constrain the flow. With the **Suppress backflow** option

$$\begin{gathered}\left(-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)-\frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right)\mathbf{n} = -\hat{p}_0\mathbf{n}\\ (-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T))\mathbf{n} = -\hat{p}_0\mathbf{n}\\ \hat{p}_0 \le p_0\end{gathered}, \tag{3-29}$$

the normal stress is adjusted to keep

$$\mathbf{u}\cdot\mathbf{n} \ge 0 \tag{3-30}$$

Equation 3-29 effectively means that the prescribed pressure is p_0 if $\mathbf{u}\cdot\mathbf{n} \ge 0$, but smaller at locations where $\mathbf{u}\cdot\mathbf{n} < 0$. This means that Equation 3-29 does not

completely prevent backflow, but the backflow is substantially reduced. Backflow is suppressed also when external forces are acting on the fluid, provided the magnitude of these forces are of the same order as the dynamic pressure at the outlet.

A pressure condition can also be applied at an inlet. In this case, either the normal stress is prescribed

$$\begin{gathered}\mathbf{n}^T\left(-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)-\frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right)\mathbf{n}=-\hat{p}_0\\ \mathbf{n}^T(-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T))\mathbf{n}=-\hat{p}_0\\ \hat{p}_0\geq p_0\end{gathered} \tag{3-31}$$

together with the tangential condition in Equation 3-28, or, a general flow direction is prescribed.

$$\begin{gathered}\mathbf{r}_\mathbf{u}^T\left(-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)-\frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right)\mathbf{n}=-\hat{p}_0(\mathbf{r}_\mathbf{u}\cdot\mathbf{n})\\ \mathbf{r}_\mathbf{u}^T(-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T))\mathbf{n}=-\hat{p}_0(\mathbf{r}_\mathbf{u}\cdot\mathbf{n})\\ \hat{p}_0\geq p_0\\ \mathbf{u}-(\mathbf{u}\cdot\mathbf{r}_\mathbf{u})\mathbf{r}_\mathbf{u}=\mathbf{0},\ \mathbf{r}_\mathbf{u}=\frac{\mathbf{d}_\mathbf{u}}{\|\mathbf{d}_\mathbf{u}\|}\end{gathered} \tag{3-32}$$

The “>” option is used with suppress backflow to have $\mathbf{u}\cdot\mathbf{n}\leq 0$ or $\mathbf{u}\cdot\mathbf{r}_\mathbf{u}\geq 0$.

For incompressible single-phase flow, it is also allowed to specify the total pressure, p_{tot}, instead of the static pressure, p_{stat}, on inlet and outlet boundaries. It is more useful, for example, in pump applications. The pressure is then prescribed at the boundaries using Bernoulli’s principle,

$$p=p_{\text{stat}}=p_{\text{tot}}-\frac{1}{2}\rho|\mathbf{u}|^2 \tag{3-33}$$

The equation is imposed with two options: **Average** and **Pointwise**.

In the first option, p_{stat} is prescribed by:

$$\mathbf{n}^T(-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T))\mathbf{n}=\mathbf{n}^T(-p_{\text{stat}}\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T))\mathbf{n} \tag{3-34}$$

where p_{tot} and $|\mathbf{u}|^2$ are averaged over the boundaries using the `aveop` operator:

$$p_{\text{stat}} = \text{aveop}(p_{\text{tot}}) - \frac{1}{2}\rho \cdot \text{aveop}(|\mathbf{u}|^2)$$

For the second option, Equation 3-33 is prescribed pointwise.

See Inlet, Outlet, Open Boundary, and No Viscous Stress for the individual node settings. Note that some modules have additional theory sections describing options available with that module.

Porous Interface

This condition properly accounts for a sudden jump in porosity ε_p across boundary between different domains, giving the corresponding jump in stress across the interface. The emergence of a boundary layer on the upstream side of the interface is also revealed, which provides modifications to the behavior of the tangential velocity near the interface. The feature helps to avoid the need to add a very thin transition region, in which $\varepsilon_{p,\text{upstream}}$ changes to $\varepsilon_{p,\text{downstream}}$ continuously, while solving the Brinkman equation in such situations. Below, '–' and '+' (used as subscripts and superscripts) refer to the upstream and downstream side of the interface, respectively.

Whatever the option for **Continuity conditions** is chosen, the velocity conditions are

$$[\rho(\mathbf{u}\cdot\mathbf{n})]\Big|_{-}^{+} = 0, \qquad \mathbf{u}_t\Big|_{-}^{+} \equiv [\mathbf{u} - (\mathbf{u}\cdot\mathbf{n})\mathbf{n}]\Big|_{-}^{+} = 0$$

That is, the mass flux and tangential velocity across the interface are constant, and $\mathbf{n}$ is assumed to be a normal pointing from '–' to '+'. **Velocity and stress** option just imposes usual stress continuity adding a correction for a possible jump in density:

$$\left[p\mathbf{n} - \mathbf{K}\mathbf{n} + \rho(\mathbf{u}\cdot\mathbf{n})\left(\left[\frac{1}{\varepsilon_p}\right]_{\text{av}}\right)^2\mathbf{u}\right]\Bigg|_{-}^{+} = 0$$

The option **Velocity and porosity-corrected stress** (default) adds a contribution due to the inertial term, which is nontrivial (gives nonzero effect) when ε_p jumps across the interface:

$$\left[p\mathbf{n} - \mathbf{K}\mathbf{n} + \rho(\mathbf{u}\cdot\mathbf{n})\left(\left[\frac{1}{\varepsilon_p}\right]_{\text{av}}\right)^2\mathbf{u} + \rho(\mathbf{u}\cdot\mathbf{n})\left(\frac{1}{2\varepsilon_p^2}\right)\mathbf{u}_{\text{av}}\right]\Bigg|_{-}^{+} = 0$$

Notice that $\left[\frac{1}{\varepsilon_p}\right]_{av} = \left(\left[\frac{1}{\varepsilon_p}\right]_- + \left[\frac{1}{\varepsilon_p}\right]_+\right)/2, \quad \mathbf{u}_{av} = (\mathbf{u}_- + \mathbf{u}_+)/2$ and so on.

Then, the **Velocity and porosity-corrected stress with loss** option has a 'pressure loss' term:

$$\left[p\mathbf{n} - \mathbf{K}\mathbf{n} + \rho(\mathbf{u}\cdot\mathbf{n})\left(\left[\frac{1}{\varepsilon_p}\right]_{av}\right)^2\mathbf{u} + \rho(\mathbf{u}\cdot\mathbf{n})\left(\frac{1}{2\varepsilon_p^2}\right)\mathbf{u}_{av}\right]\Bigg|_-^+ + p^{(\mathrm{loss})}\mathbf{n} = 0$$

This loss occurs in the downstream direction. Its mechanism is similar to the mechanism of common engineering 'total pressure loss'. Indeed, 'expansion' and 'contraction' across the interface experienced by the flow on the microscopic level (due to increasing or decreasing porosity, ε_p, respectively), are roughly equivalent to expansion and contraction of flow in a pipe with geometrical variations. Accordingly, it is assumed that only the normal velocity component is responsible for the loss. In the case of normal flow and negligible viscous term the pipe-analogy is quite exact.

Subsequently, **Pressure loss model** should be specified. Choosing **User-defined loss coefficients** requires values of **Expansion loss coefficient** and **Contraction loss coefficient** ($K_{exp} = 1$ and $K_{contr} = 0.5$ are default values). The resulting losses on the 'expansion' and 'contraction' boundaries are:

$$p^{(\mathrm{loss,expansion})} = K_{\mathrm{exp}}\left(\left(\frac{\rho(\mathbf{u}\cdot\mathbf{n})^2}{2\varepsilon_p^2}\right)_-\right),$$

$$p^{(\mathrm{loss,contraction})} = K_{\mathrm{contr}}\left(\frac{\rho(\mathbf{u}\cdot\mathbf{n})^2}{2\varepsilon_p^2}\right)_+$$

Borda–Carnot option results in the following losses:

$$p^{(\mathrm{loss,expansion})} = \frac{\rho_{av}}{2}\left(\left[\frac{(\mathbf{u}\cdot\mathbf{n})}{\varepsilon_p}\right]_+ - \left[\frac{(\mathbf{u}\cdot\mathbf{n})}{\varepsilon_p}\right]_-\right)^2,$$

$$p^{(\mathrm{loss,contraction})} = \frac{1}{2}\left(\frac{\rho(\mathbf{u}\cdot\mathbf{n})^2}{\varepsilon_p^2}\right)_+\left(\frac{1}{c_{vc}} - 1\right)^2$$

and requires to choose **Vena contracta model**. The **User defined** option asks for value of **Vena contracta coefficient** ($c_{vc} = 0.5$ by default). **Weisbach** option computes the coefficient based on the ratio of porosities across the interface:

$$c_{vc} = c_{vc,ll} + (1 - c_{vc,ll})\left(\frac{\varepsilon_{p,+}}{\varepsilon_{p,-}}\right)^{n_{vc}}$$

and requires inputs for **Lower limit** and **Exponent** ($c_{vc,ll} = 0.63$ and $n_{vc} = 3$ are default values).

Although the velocity conditions formally look the same for all **Continuity conditions** options, the latter two (containing the inertial correction due to the porosity jump) lead to an extra nontrivial effect. Namely, the tangential velocity exponentially evolves over a boundary layer formed on the upstream side of the interface boundary. This boundary layer has a characteristic length equal to

$$l_- = \frac{\mu\varepsilon_{p,-}}{\rho(\mathbf{u}\cdot\mathbf{n})}$$

The ratio of the tangential velocities right after the interface ('downstream') and outside the boundary layer ('upstream infinity') is

$$\frac{|\mathbf{u}_{t,+}|}{|\mathbf{u}_{t,\text{upstream infinity}}|} = \frac{2\varepsilon_{p,+}/\varepsilon_{p,-}}{\varepsilon_{p,+}/\varepsilon_{p,-} + \varepsilon_{p,-}/\varepsilon_{p,+}}$$

In terms of the interstitial velocity, $\mathbf{u}^{(i)} = \mathbf{u}/\varepsilon_p$, this results in:

$$\frac{|\mathbf{u}^{(i)}{}_{t,+}|}{|\mathbf{u}^{(i)}{}_{t,\text{upstream infinity}}|} = \frac{2}{\varepsilon_{p,+}/\varepsilon_{p,-} + \varepsilon_{p,-}/\varepsilon_{p,+}} \leq 1$$

Obviously, tangential component of the interstitial kinetic energy is lost across the interface. For low viscosity and high normal-flow component, when l_u is much lower than l_{geom} (the characteristic geometry length) there are apparent variations in $\mathbf{u}_t$ and $\mathbf{u}^{(i)}{}_t$ in a thin boundary layer on the upstream side of the interface. However, for the cases with high viscosity or nearly interface-parallel flow, l_u is much larger than l_{geom}, and any variations in $\mathbf{u}_t$ and $\mathbf{u}^{(i)}{}_t$ are virtually invisible.

Notice that the feature does not take into account possible underresolved porous scale, as is described in Theory for the Free and Porous Media Flow, Darcy Interface.

Mass Sources for Fluid Flow

There are two types of mass sources in a Single-Phase Flow interface: point sources and line sources.

	These features require at least one of the following licenses: Battery Design Module, CFD Module, Chemical Reaction Engineering Module, Corrosion Module, Electrochemistry Module, Electrodeposition Module, Fuel Cell & Electrolyzer Module, Microfluidics Module, Pipe Flow Module, Polymer Flow Module, or Subsurface Flow Module.

POINT SOURCE

A point source is theoretically formed by taking a mass injection/ejection, $\dot{Q}$ (SI unit: kg/(m^3·s)), in a small volume δV and then letting the size of the volume tend to zero while keeping the total mass flux constant. Given a point source strength, $\dot{q}_\mathrm{p}$ (SI unit: kg/s), this can be expressed as

$$\lim_{\delta V \to 0} \int_{\delta V} \dot{Q} = \dot{q}_\mathrm{p} \tag{3-35}$$

An alternative way to form a point source/sink is to assume that mass is injected/extracted through the surface of a small object. Letting the object surface area tend to zero while keeping the mass flux constant, results in the same point source. For this alternative approach, effects resulting from the physical object volume, such as drag and fluid displacement, need to be neglected.

The weak contribution

$$\dot{q}_\mathrm{p}\mathrm{test}(p)$$

is added to a point in the geometry. As can be seen from Equation 3-35, $\dot{Q}$ must tend to plus or minus infinity as δV tends to zero. This means that in theory the pressure also tends to plus or minus infinity.

Observe that "point" refers to the physical representation of the source. A point source can therefore only be added to points in 3D components and to points on the symmetry axis in 2D axisymmetry components. Other geometrical points in 2D components represent physical lines.

The finite element representation of Equation 3-35 corresponds to a finite pressure in a point with the effect of the point source spread out over a region around the point.

The size of the region depends on the mesh and on the strength of the source. A finer mesh gives a smaller affected region, but also a more extreme pressure value. It is important not to mesh too finely around a point source since the resulting pressure can result in unphysical values for the density, for example. It can also have a negative effect on the condition number for the equation system.

LINE SOURCE

A line source can theoretically be formed by assuming a source of strength $\dot{Q}$ (SI unit: kg/(m^3·s)), located within a tube with cross-sectional area δS and then letting δS tend to zero, while keeping the total mass flux per unit length constant. Given a line source strength, $\dot{q}_l$ (SI unit: kg/(m·s)), this can be expressed as

$$\lim_{\delta S \to 0} \int_{\delta S} \dot{Q} = \dot{q}_l \tag{3-36}$$

As in the point source case, an alternative approach is to assume that mass is injected/extracted through the surface of a small object. This results in the same mass source, but requires that effects on the fluid resulting from the physical object volume are neglected.

The weak contribution

$$\dot{q}_l \mathrm{test}(p)$$

is added to lines in 3D or to points in 2D (which represent cut-through views of lines). Line sources can also be added to the axisymmetry line in 2D axisymmetry components. It cannot, however, be added to geometrical lines in 2D because they represent physical planes.

As with a point source, it is important not to mesh too finely around the line source.

	For feature node information, see Line Mass Source and Point Mass Source in the *COMSOL Multiphysics Reference Manual*.

For the Reacting Flow in Porous Media, Diluted Species interface, which is available with the CFD Module, Chemical Reaction Engineering Module, or Battery Design Module, these shared physics nodes are renamed as follows:

- The **Line Mass Source** node is available as two nodes, one for the fluid flow (**Fluid Line Source**) and one for the species (**Species Line Source**).
- The **Point Mass Source** node is available as two nodes, one for the fluid flow (**Fluid Point Source**) and one for the species (**Species Point Source**).

Numerical Stability — Stabilization Techniques for Fluid Flow

The momentum equation (Equation 3-10 or Equation 3-12) is a (nonlinear) convection-diffusion equation. Such equations can easily become unstable if discretized using the Galerkin finite element method. Stabilized finite element methods are usually necessary in order to obtain physical solutions. The stabilization settings are found in the main Fluid Flow interface features. To display this section, click the **Show More Options** button ( ) and select **Stabilization** in the **Show More Options** dialog.

There are three types of stabilization methods available for Navier–Stokes — *streamline diffusion*, *crosswind diffusion*, and *isotropic diffusion*. Streamline diffusion and crosswind diffusion are consistent stabilization methods, whereas isotropic diffusion is an inconsistent stabilization method.

For optimal functionality, the exact weak formulations of and constants in the streamline diffusion and crosswind diffusion methods depend on the order of the shape functions (basis functions) for the elements. The values of constants in the streamline diffusion and crosswind diffusion methods follow Ref. 5 and Ref. 6.

STREAMLINE DIFFUSION

For strongly coupled systems of equations, the streamline diffusion method must be applied to the system as a whole rather than to each equation separately. These ideas were first explored by Hughes and Mallet (Ref. 8) and were later extended to Galerkin least-squares (GLS) applied to the Navier–Stokes equations (Ref. 9). This is the streamline diffusion formulation that COMSOL Multiphysics supports.

Streamline diffusion is active by default because it is necessary when convection is dominating the flow.

The governing equations for incompressible flow are subject to the Babuška–Brezzi condition, which states that the shape functions (basis functions) for pressure must be of lower order than the shape functions for velocity. If the incompressible Navier–Stokes equations are stabilized by streamline diffusion, it is possible to use equal-order interpolation. Hence, streamline diffusion is necessary when using first-order elements for both velocity and pressure. This applies also if the model is solved using geometric multigrid (either as a solver or as a preconditioner) and at least one multigrid hierarchy level uses linear Lagrange elements.

CROSSWIND DIFFUSION

Crosswind diffusion can also be formulated for systems of equations, and when applied to the Navier–Stokes equations it becomes a shock-capturing operator. COMSOL Multiphysics supports the formulation in Ref. 9 with a shock-capturing viscosity of the Hughes–Mallet type Ref. 8.

Incompressible flows do not contain shock waves, but crosswind diffusion is still useful for introducing extra diffusion in sharp boundary layers and shear layers that otherwise would require a very fine mesh to resolve.

Crosswind diffusion is active by default as it makes it easier to obtain a solution even if the problem is fully resolved by the mesh. Crosswind diffusion also enables the iterative solvers to use inexpensive presmoothers. If crosswind diffusion is deactivated, more expensive preconditioners must be used instead.

STABILIZATION TIME SCALES

The time-scale tensor for time-dependent problems should in theory depend on a time-scale that many references just set to the time-step taken by the time-solver, Δt (see, for example, Ref. 9 and Ref. 10). This simple approach does not, however, necessarily reflect on the actual time-scales in the physics. A typical example is reacting flows where the time step is often guided by fast reactions, while the flow develops relatively slowly. The COMSOL Multiphysics software can therefore replace Δt^2 in the time-scale tensor with measures of type $(1/(\Delta\tilde{t})^2)^{-1}$, which are calculated from projections of weak expressions in a fashion similar to those in Ref. 11. These measures of the time scale are used when **Use dynamic subgrid time scale** is activated.

The **Limit small time steps effect on stabilization time scale** option can be used to ramp down the time-step contribution in the stabilization when the time step becomes much smaller than the convective and diffusive time scales. This option prevents loss of pressure stabilization at such small time steps.

ISOTROPIC DIFFUSION

Isotropic diffusion adds diffusion to the Navier–Stokes equations. Isotropic diffusion significantly reduces the accuracy of the solution but does a very good job at reducing oscillations. The stability of the continuity equation is not improved.

	Numerical Stabilization and Iterative in the *COMSOL Multiphysics Reference Manual*

Solvers for Laminar Flow

The Navier–Stokes equations constitute a nonlinear equation system. A nonlinear solver must hence be applied to solve the problem. The nonlinear solver iterates to reach the final solution. In each iteration, a linearized version of the nonlinear system is solved using a linear solver. In the time-dependent case, a time marching method must also be applied. The default suggestions for each of these solver elements are discussed below.

NONLINEAR SOLVER

The nonlinear solver method depends on if the model solves a stationary or a time-dependent problem.

Stationary Solver

In the stationary case, a fully coupled, damped Newton method is applied. The initial damping factor is low since a full Newton step can be harmful unless the initial values are close to the final solution. The nonlinear solver algorithm automatically regulates the damping factor in order to reach a converged solution.

For advanced models, the automatically damped Newton method might not be robust enough. A pseudo time-stepping algorithm can then be invoked. See Pseudo Time Stepping for Laminar Flow Models.

Time-Dependent Solver

In the time-dependent case, the initial guess for each time step is (loosely speaking) the previous time step, which is a very good initial value for the nonlinear solver. The automatic damping algorithm is then not necessary. The damping factor in the Newton method is instead set to a constant value slightly smaller than one. Also, for the same reason, it suffices to update the Jacobian once per time step.

It is seldom worth the extra computational cost to update the Jacobian more than once per time step. For most models it is more efficient to restrict the maximum time step or possibly lower the damping factor in the Newton method.

LINEAR SOLVER

The linearized Navier–Stokes equation system has saddle point character, unless the density depends on the pressure. This means that the Jacobian matrix has zeros on the diagonal. Even when the density depends on the pressure, the equation system effectively shares many numerical properties with a saddle point system.

For small 2D and 3D models, the default solver suggestion is a direct solver. Direct solvers can handle most nonsingular systems and are very robust and also very fast for small models. Unfortunately, they become slow for large models and their memory requirement scales as somewhere between $N^{1.5}$ and N^2, where N is the number of degrees of freedom in the model. The default suggestion for large 2D and 3D models is therefore the iterative GMRES solver. The memory requirement for an iterative solver optimally scales as N.

GMRES is accelerated by a multigrid method, per default the smoothed aggregation algebraic multigrid (SAAMG) method. The cost of SAAMG is typically very low compared to the number of GMRES iterations necessary if no multigrid method is used. As the name implies, SAAMG builds its coarser meshes algebraically, so the application requires no additional meshes in order to employ SAAMG. In contrast, the geometric multigrid (GMG) method requires actual meshes. If a sufficient number of multigrid levels can be constructed, GMG is often faster than SAAMG. GMG is also superior for cluster computations and for shared-memory computations with many cores. When the default linear solver is GMRES, an optional, but deactivated, linear solver node is available where GMRES is accelerated by GMG.

Multigrid methods need smoothers, but the saddle point character of the linear system restricts the number of applicable smoothers. The choices are further restricted by the anisotropic meshes frequently encountered in fluid-flow problems. The efficiency of the smoothers is highly dependent on the numerical stabilization. Iterative solvers perform at their best when both Streamline Diffusion and Crosswind Diffusion are active.

The default smoother for P1+P1 elements is SCGS. This is an efficient and robust smoother specially designed to solve saddle point systems on meshes that contain anisotropic elements. The SCGS smoother works well even without crosswind diffusion. SCGS can sometimes work for higher-order elements, especially if **Method** in the SCGS settings is set to **Mesh element lines**. But there is no guarantee for this, so the

default smoother for higher order elements is an SOR Line smoother. SOR Line handles mesh anisotropy but does not formally address the saddle point character. It does, however, function in practice provided that streamline diffusion and crosswind diffusion are both active.

A different kind of saddle point character can arise if the equation system contains ODE variables. Some advanced boundary conditions can add equations with such variables. These variables must be treated with the Vanka algorithm. SCGS includes an option to invoke Vanka. Models with higher-order elements must apply SCGS or use the Vanka smoother. The latter is the default suggestion for higher-order elements, but it does not work optimally for anisotropic meshes.

TIME-DEPENDENT SOLVERS

The default time-dependent solver for Navier–Stokes is the BDF method with maximum order set to two. Higher BDF orders are not stable for transport problems in general nor for Navier–Stokes in particular.

BDF methods have been used for a long time and are known for their stability. However, they can have severe damping effects, especially the lower-order methods. Hence, if robustness is not an issue, a model can benefit from using the generalized-α method instead. Generalized-α is a solver that has properties similar to those of the second-order BDF solver but it is much less diffusive.

Both BDF and generalized-α are per default set to automatically adjust the time step. While this works well for many models, extra efficiency and accuracy can often be gained by specifying a maximum time step. It is also often beneficial to specify an initial time step to make the solver progress smoothly in the beginning of the time series.

In the *COMSOL Multiphysics Reference Manual:*

- Time-Dependent Solver
- Multigrid, Direct, Iterative, SCGS, SOR Line, and Vanka
- Stationary Solver

Pseudo Time Stepping for Laminar Flow Models

A stationary formulation has per definition no time derivatives and Equation 3-12 reduces to:

$$\rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot[-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)]+\mathbf{F} \tag{3-37}$$

Solving Equation 3-37 requires a starting guess that is close enough to the final solution. If no such guess is at hand, the fully transient problem can be solved instead. This is, however, a rather costly approach in terms of computational time. An intermediate approach is to add a fictitious time derivative to Equation 3-37:

$$\rho\frac{\mathbf{u}-\mathrm{nojac}(\mathbf{u})}{\Delta\tilde{t}}+\rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot[-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)]+\mathbf{F}$$

where $\Delta\tilde{t}$ is a *pseudo time step*. Since $\mathbf{u}-\mathtt{nojac}(\mathbf{u})$ is always zero, this term does not affect the final solution. It does, however, affect the discrete equation system and effectively transforms a nonlinear iteration into a step of size $\Delta\tilde{t}$ of a time-dependent solver.

Pseudo time stepping is not active per default. The pseudo time step $\Delta\tilde{t}$ can be chosen individually for each element based on the local CFL number:

$$\Delta\tilde{t} = \mathrm{CFL}_{\mathrm{loc}}\frac{h}{|\mathbf{u}|}$$

where h is the mesh cell size. A small CFL number means a small time step. It is practical to start with a small CFL number and gradually increase it as the solution approaches steady state.

If the automatic expression for $\mathrm{CFL}_{\mathrm{loc}}$ is set to the built-in variable `CFLCMP`, then the automatic setting suggests a PID regulator for the pseudo time step in the default solver. The PID regulator starts with a small CFL number and increases $\mathrm{CFL}_{\mathrm{loc}}$ as the solution comes closer to convergence.

The default manual expression is

$$\begin{gathered}1.3^{\min(\mathrm{niterCMP},\,9)}+\\ \mathrm{if}(\mathrm{niterCMP}>20,\,9\cdot 1.3^{\min(\mathrm{niterCMP}-20,\,9)},\,0)+\\ \mathrm{if}(\mathrm{niterCMP}>40,\,90\cdot 1.3^{\min(\mathrm{niterCMP}-40,\,9)},\,0)\end{gathered} \tag{3-38}$$

The variable `niterCMP` is the nonlinear iteration number. It is equal to one for the first nonlinear iteration. $\mathrm{CFL}_{\mathrm{loc}}$ starts at 1.3 and increases by 30% each iteration until it reaches $1.3^9 \approx 10.6$. It remains there until iteration number 20 at which it starts to increase until it reaches approximately 106. A final increase after iteration number 40

then takes it to 1060. Equation 3-38 can, for some advanced flows, increase $\mathrm{CFL}_{\mathrm{loc}}$ too slowly or too quickly. $\mathrm{CFL}_{\mathrm{loc}}$ can then be tuned for the specific application.

For details about the CFL regulator, see Pseudo Time Stepping in the *COMSOL Multiphysics Reference Manual*.

Nitsche Constraints

Some boundary conditions are implemented using Nitsche constraints. These boundary conditions include

- Wall — Slip, sliding walls, and moving walls (that is, walls with nonzero translational velocity).
- Periodic Flow Condition
- Flow Continuity

The formulation used in the Fluid Flow interfaces in single-phase flow interfaces corresponds to the Symmetric Interior Penalty Galerkin method (SIPG). The SIPG method can be regarded to satisfy the boundary conditions in an integral sense rather than pointwise. More information on SIPG can be found in Ref. 15.

In particular, the SIPG formulation includes a penalty parameter that must be large enough for the formulation to be coercive. The higher the value, the better the boundary condition is fulfilled, but a too high value results in an ill-conditioned equation system. The penalty parameter is implemented according to Ref. 16.

Particle Tracing in Fluid Flow

The Particle Tracing Module is available to assist with these types of modeling problems.

It is possible to model particle tracing with COMSOL Multiphysics provided that the impact of the particles on the flow field is negligible. First compute the flow field, and then, as an analysis step, calculate the motion of the particles. The motion of a particle is defined by Newton's second law

$$m\frac{d^2\mathbf{x}}{dt^2} = \mathbf{F}\left(t, \mathbf{x}, \frac{d\mathbf{x}}{dt}\right)$$

where $\mathbf{x}$ is the position of the particle, m the particle mass, and $\mathbf{F}$ is the sum of all forces acting on the particle. Examples of forces acting on a particle in a fluid are the drag force, the buoyancy force, and the gravity force. The drag force represents the force that a fluid exerts on a particle due to a difference in velocity between the fluid and the particle. It includes the viscous drag, the added mass, and the Basset history term. Several empirical expressions have been suggested for the drag force. One of those is the one proposed by Khan and Richardson (Ref. 13). That expression is valid for spherical particles for a wide range of particle Reynolds numbers. The particle Reynolds number is defined as

$$\mathrm{Re}_p = \frac{|\mathbf{u} - \mathbf{u}_p| 2r\rho}{\mu}$$

where $\mathbf{u}$ is the velocity of the fluid, $\mathbf{u}_p$ the particle velocity, r the particle radius, ρ the fluid density, and μ the dynamic viscosity of the fluid. The empirical expression for the drag force according to Khan and Richardson is

$$\mathbf{F} = \pi r^2 \rho |\mathbf{u} - \mathbf{u}_p| (\mathbf{u} - \mathbf{u}_p)[1.84\mathrm{Re}_p^{-0.31} + 0.293\mathrm{Re}_p^{0.06}]^{3.45}$$

The model *Flow Past a Cylinder* (Application Library path **COMSOL_Multiphysics/Fluid_Dynamics/cylinder_flow**) demonstrates how to add and set up particle tracing in a plot group using the **Particle Tracing with Mass** node. It uses the predefined Khan–Richardson model for the drag force and neglects gravity and buoyancy forces.

References for the Single-Phase Flow, Laminar Flow Interfaces

1. G.G. Stokes, *Trans. Camb. Phil. Soc.*, vol. 8, pp. 287–305, 1845.

2. P.M. Gresho and R.L. Sani, *Incompressible Flow and the Finite Element Method, Volume 2: Isothermal Laminar Flow*, John Wiley & Sons, 2000.

3. G.K. Batchelor, *An Introduction To Fluid Dynamics*, Cambridge University Press, 1967.

4. R.L. Panton, *Incompressible Flow*, 2nd ed., John Wiley & Sons, 1996.

5. I. Harari and T.J.R. Hughes, "What are *C* and *h*? Inequalities for the Analysis and Design of Finite Element Methods," *Comput. Methods Appl. Mech. Eng.*, vol. 97, pp. 157–192, 1992.

6. Y. Bazilevs, V.M. Calo, T.E. Tezduyar, and T.J.R. Hughes, "*YZβ* Discontinuity Capturing for Advection-dominated Processes with Application to Arterial Drug Delivery," *Int. J. Num. Meth. Fluids*, vol. 54, pp. 593–608, 2007.

7. R.B. Bird, W.E. Stewart, and E.N. Lightfoot, *Transport Phenomena*, 2nd ed., John Wiley & Sons, 2007.

8. T.J.R. Hughes and M. Mallet, "A New Finite Element Formulation for Computational Fluid Dynamics: III. The Generalized Streamline Operator for Multidimensional Advective-Diffusive System," *Comput. Methods Appl. Mech. Eng.*, vol. 58, pp. 305–328, 1986.

9. G. Hauke and T.J.R. Hughes, "A Unified Approach to Compressible and Incompressible Flows," *Comput. Methods Appl. Mech. Eng.*, vol. 113, pp. 389–395, 1994.

10. G. Hauke, "Simple Stabilizing Matrices for the Computation of Compressible Flows in Primitive Variables", *Comput. Methods Appl. Mech. Eng.*, vol. 190, pp. 6881–6893, 2001.

11. M.-C. Hsu, Y. Bazilevs, V.M. Cali, T.E. Tezduyar, and T.J.R. Hughes, "Improving stability of stabilized and multiscale formulations in flow simulations at small time steps," *Comput. Methods Appl. Mech. Eng.*, vol. 199, pp. 828–840, 2010.

12. D.J. Tritton, *Physical Fluid Dynamics*, 2nd ed., Oxford University Press, 1988.

13. J.M. Coulson and J.F. Richardson, "Particle Technology and Separation Processes," *Chemical Engineering, Volume 2*, Butterworth-Heinemann, 2002.

14. J.L. Guermond, P. Minev, and J. Shen, "An overview of projection methods for incompressible flows," *Comput. Methods Appl. Mech. Eng.*, vol. 195, pp. 6011–6045, 2006.

15. B. Rivière, *Discontinuous Galerkin Methods for Solving Elliptic and Parabolic Equations*, SIAM, 2008.

16. Y. Epshteyn and B. Rivière, "Estimation of penalty parameters for symmetric interior penalty Galerkin methods," *J. Comput. Appl. Math.*, vol. 206, pp. 843–872, 2007.

17. G. Kariadakis, A. Beskok, and N. Aluru, *Microflows and Nanoflows*, Springer Science and Business Media, 2005.

18. R.P. Chhabra and J.F. Richardson, *Non-Newtonian Flow and Applied Rheology*, 2nd ed., Elsevier, 2008.

19. Y. Bazilevs and T.J.R. Hughes, "Weak imposition of Dirichlet boundary conditions in fluid mechanics," *Comput. Fluids*, vol. 36, pp. 12–26, 2007.

20. G. Kariadakis, A. Beskok, and N. Aluru, *Microflows and Nanoflows*, Springer Science and Business Media, 2005.

Theory for the Potential Flow Interface

The theory for the Incompressible Potential Flow interface is described in the following section.

General Incompressible Potential Flow Theory

The Incompressible Potential Flow interface is used to simulate irrotational, inviscid, and incompressible flow. The continuity equation for incompressible flow can be expressed as a divergence-free constraint for the velocity

$$\nabla \cdot \mathbf{u} = 0 \tag{3-39}$$

Moreover, irrotational flow is described as

$$\nabla \times \mathbf{u} = 0 \tag{3-40}$$

As the curl of the gradient of a scalar field is zero by definition, the velocity can be approximated as the gradient of a scalar velocity potential, ϕ,

$$\mathbf{u} = -\nabla\phi \tag{3-41}$$

so that Equation 3-39 and Equation 3-41 result in the Laplace equation

$$-\nabla \cdot \nabla\phi = 0 \tag{3-42}$$

The local gauge pressure can be obtained from Bernoulli's equation

$$p = p_{\mathrm{Tot}} - \frac{\rho}{2}\|\nabla\phi\|^2 \tag{3-43}$$

where

$$p_{\mathrm{Tot}} = \frac{\rho}{2}U_{\mathrm{scale}}^2 \tag{3-44}$$

and U_{scale} is the user-defined free-stream velocity.

4

Multiphase Flow, Two-Phase Flow Interfaces

There are several Fluid Flow interfaces available with the Microfluidics Module. These are found under the **Fluid Flow** > **Multiphase Flow** branch ( ) when adding a physics interface. See Modeling Microfluidic Fluid Flows to help select the physics interface to use.

In this chapter:

- The Laminar Two-Phase Flow, Level Set and Laminar Two-Phase Flow, Phase Field Interfaces
- The Laminar Three-Phase Flow, Phase Field Interface
- The Laminar Two-Phase Flow, Moving Mesh Interface
- Theory for the Level Set and Phase Field Interfaces
- Theory for the Three-Phase Flow, Phase Field Interface
- Theory for the Two-Phase Flow, Moving Mesh Interface

The Laminar Two-Phase Flow, Level Set and Laminar Two-Phase Flow, Phase Field Interfaces

This section includes the following topics:

- The Laminar Two-Phase Flow, Level Set Interface
- The Two-Phase Flow, Level Set Coupling Feature
- The Wetted Wall Coupling Feature
- The Interior Wetted Wall Coupling Feature
- The Laminar Two-Phase Flow, Phase Field Interface
- The Two-Phase Flow, Phase Field Coupling Feature
- Domain, Boundary, Point, and Pair Nodes for the Laminar Flow, Two-Phase, Level Set and Phase Field Interfaces

	Mathematics, Moving Interfaces

The Laminar Two-Phase Flow, Level Set Interface

The **Laminar Two-Phase Flow, Level Set** interface ( ) found under the **Multiphase Flow** > **Two-Phase Flow, Level Set** branch ( ), is a multiphysics interface designed to track the interface between two immiscible fluids. The flow is assumed to be laminar, that is, to be of low to moderate Reynolds number. The fluids can be incompressible or compressible.

When adding the **Laminar Two-Phase Flow, Level Set** multiphysics interface, a **Laminar Flow** and a **Level Set** interface are added to the Model Builder. In addition, a multiphysics coupling feature, The Two-Phase Flow, Level Set Coupling Feature, is added automatically under the **Multiphysics** node. The Wetted Wall Coupling Feature is also added, but with empty selection. Other **Wetted Wall** multiphysics coupling features and The Interior Wetted Wall Coupling Feature can be added when needed to model walls.

Simulations using the Laminar Two-Phase Flow, Level Set interface are always time-dependent since the position of an interface is almost always dependent of its history.

INTERFACE PROPERTIES

Discretization

By default the fluid flow discretization is set to **P1+P1**, and the level set discretization is set to **Linear**. This combination provides exact conservation of the integral of the level set variable when using the nonconservative form of the level set equation.

- Theory for the Level Set and Phase Field Interfaces
- Theory for the Single-Phase Flow Interfaces

The Two-Phase Flow, Level Set Coupling Feature

The **Laminar Two-Phase Flow, Level Set** ( ) and **Turbulent Two-Phase Flow, Level Set** ( ) interfaces contain a multiphysics coupling feature, **Two-Phase Flow, Level Set**, which is added automatically.

The **Two-Phase Flow, Level Set** multiphysics coupling feature defines the density and dynamic viscosity of the fluid used in the **Laminar Flow** interface, and it defines the surface tension on the interface in form of a volume force used in the momentum equation. It also enables the **Level Set** interface to use the velocity field calculated from the **Laminar Flow** interface to transport the interface.

SETTINGS

The **Label** is the default multiphysics coupling feature name.

The **Name** is used primarily as a scope prefix for variables defined by the coupling node. Refer to such variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different coupling nodes or physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first multiphysics coupling feature **Two-Phase Flow, Level Set** in the model) is `tpf1`.

DOMAIN SELECTION

When nodes are added from the context menu, you can select **All domains** (the default) or select **Manual** from the **Selection** list to choose specific domains.

COUPLED INTERFACES

This section controls which individual interfaces are coupled by the current coupling feature. If a physics interface is deleted and then added to the model again, then in order to reestablish the coupling, you need to choose the correct physics interface again from the **Fluid flow** or **Moving interfaces** lists.

MODEL INPUTS

Fluid properties of each phase, such as density, viscosity, or the surface tension coefficient, can be defined through user inputs, variables, or by selecting a material. For the latter option, additional inputs, for example temperature or pressure, may be required to define these properties.

Temperature

By default, the **Temperature** model input is set to **Common model input**, and the temperature is controlled from Default Model Inputs under **Global Definitions** or by a locally defined Model Input. If a Heat Transfer interface is included in the component, it controls the temperature **Common model input**. Alternatively, the temperature field can be selected from another physics interface. All physics interfaces have their own tags (**Name**). For example, if a Heat Transfer in Fluids interface is included in the component, the **Temperature (ht)** option is available for T.

You can also select **User defined** from the **Temperature** model input in order to manually prescribe T.

Absolute Pressure

This input appears when a material requires the absolute pressure as a model input. The default **Absolute pressure** p_A is $p + p_{\text{ref}}$, where p is the dependent pressure variable from the Navier–Stokes or RANS equations, and p_{ref} is from the user input defined at the fluid flow physics interface level.

The **Absolute pressure** field can be edited by clicking **Make All Model Inputs Editable** ( ) and entering the desired value in the input field.

	Model Inputs and Multiphysics Couplings in the *COMSOL Multiphysics Reference Manual*

MATERIAL PROPERTIES

The effective density and dynamic viscosity can either be **Locally defined** or picked up from a Multiphase Material. When the properties are defined locally, provide the properties for each phase in the respective fluid properties section, and the averaging method in the advanced settings section. If a multiphase material is used, these settings are controlled from the material. Using a multiphase material is advantageous for models coupling two-phase flow with other physics interfaces, such as Heat Transfer in Fluids or Electrostatics. In such cases, the multiphase material can ensure that the effective material properties for these physics interfaces are averaged using the volume fraction from the Level Set physics interface.

Click the **Go to Material** button ( ) to move to the selected material node. Click the **Add Multiphase Material** button ( ) to add a multiphase material with two phases. The added material then becomes the one selected in the **Multiphase Material** list.

	Multiphase Material in the *COMSOL Multiphysics Reference Manual*

FLUID PROPERTIES

A **Fluid Properties** section will be available per phase if the **Material Properties** are set to **Locally defined**. Use the corresponding section to specify the properties of the two fluids. The fluids are denoted **Fluid 1** and **Fluid 2**, respectively.

To specify the properties of **Fluid 1** from a material, select the appropriate material in the **Fluid 1** list. Also make sure that the **Density of fluid 1** ρ_1 and **Dynamic viscosity of fluid 1** μ_1 are both set to **From Material**.

The density in a material can depend on temperature and/or pressure and these dependencies are automatically replaced by p_{ref} and T_{ref} for incompressible flows (as specified by the **Compressibility** setting of the fluid flow interface).

The non-Newtonian Power law, Carreau, Bingham–Papanastasiou, Herschel–Bulkley–Papanastasiou, and Casson–Papanastasiou models can alternatively be used to specify the dynamic viscosities of the two fluids.

To instead apply a variable or expression for the density or dynamic viscosity for Fluid A, select **User defined** in the **Density of fluid 1** ρ_1 or the **Dynamic viscosity of fluid 1** μ_1 list and enter the expression in the corresponding text field.

Similarly, the properties of **Fluid 2** can be specified. The default material is set to **None**.

⚠	Care should be taken when using the **Domain Material** setting for the material properties for Fluid 1 and Fluid 2. The material properties are obtained from the domain irrespective of the location of the interface. If two different materials are selected in domains 1 and 2, with the phase boundary initially coincident with the domain boundary, the model has convergence issues once the phase boundary moves away from the domain boundary. This is because a density discontinuity and a viscosity discontinuity occurs at the boundary separating the two fluids. For this reason, selecting the material directly is recommended when setting the material properties for Fluid 1 and Fluid 2.

ADVANCED SETTINGS

If the **Material Properties** are set to **Locally defined**, you can specify the averaging method for density and dynamic viscosity in this section. The default method for **Density averaging** and **Viscosity averaging** is **Volume average**. In addition to the default method, **Density averaging** can be set to **Heaviside function** or **Harmonic volume average**, while **Viscosity averaging** can be set to **Heaviside function**, **Harmonic volume average**, **Mass average**, or **Harmonic mass average**. When a **Heaviside function** is used, enter a value for the corresponding mixing parameter, l_ρ or l_μ.

SURFACE TENSION

Select the **Include surface tension force in momentum equation** checkbox to include the surface tension force in the momentum equation. The surface tension force is not added to porous domains.

Select a **Surface tension coefficient** σ (SI unit: N/m):

- To use a predefined expression, select **Library coefficient, liquid/gas interface** or **Library coefficient, liquid/liquid interface**. Then select an option from the list that displays below (for example, **Water/Air** or **Glycerol/Air**). The predefined correlations are based on the data in Ref. 7, Ref. 8, and Ref. 9.
- For **User defined** enter a value or expression for the surface tension coefficient σ (SI unit: N/m).

The Wetted Wall Coupling Feature

The **Laminar Two-Phase Flow, Level Set** ( ) interface contains an optional multiphysics coupling boundary feature, **Wetted Wall**. It is an exclusive feature that overrides the **Wall** feature in the Laminar interface as well as the **No Flow** feature in the Level Set interface. It cannot be used in boundaries that have a **Flow Continuity** feature in the flow physics interface or a **Continuity** feature in the level set physics interface.

The **Wetted Wall** boundary condition is suitable for walls in contact with the fluid-fluid interface. When this boundary condition is used, the fluid-fluid interface can move along the wall.

For laminar flow, this boundary condition enforces the no-penetration condition $\mathbf{u} \cdot \mathbf{n}_{\text{wall}} = 0$ and adds a tangential stress on the form

$$\mathbf{K}_{\text{nt}} = -\frac{\mu}{\beta}\mathbf{u}$$

where $\mathbf{K}_{\text{nt}} = \mathbf{K}_{\text{n}} - (\mathbf{K}_{\text{n}} \cdot \mathbf{n}_{\text{wall}})\mathbf{n}_{\text{wall}}$, $\mathbf{K}_{\text{n}} = \mathbf{K}\mathbf{n}_{\text{wall}}$, and $\mathbf{K}$ is the viscous stress tensor. β is the slip length. For numerical calculations, a suitable choice is $\beta = h$, where h is the mesh element size. The boundary condition does not set the tangential velocity component to zero. However, the extrapolated tangential velocity component is 0 at a distance β outside the wall (see Figure 4-1).If the surface tension force is included in the momentum equation in The Two-Phase Flow, Level Set Coupling Feature, the **Wetted Wall** boundary condition also adds the following boundary force to enforce the contact angle:

$$\mathbf{F}_{\theta} = \sigma\delta(\mathbf{n}_{\text{wall}} \cdot \mathbf{n} - \cos\theta_{\text{w}})\mathbf{n}$$

The contact angle θ_{w} is defined as the angle between the fluid interface and the wall (see Figure 4-1). For more information, see Ref. 4 and Ref. 5. Note that the contact angle is not enforced on boundaries adjacent to porous domains.

The contact angle θ_{w} can be defined directly or from Young's equation, which considers the components of the forces in the plane of the surface:

$$\sigma\cos(\theta_{\text{w}}) + \gamma_{s2} = \gamma_{s1} \tag{4-1}$$

where γ_{s1} is the surface energy density on the fluid 1 — solid (wall) interface and γ_{s2} is the surface energy density on the fluid 2 — solid (wall) interface.

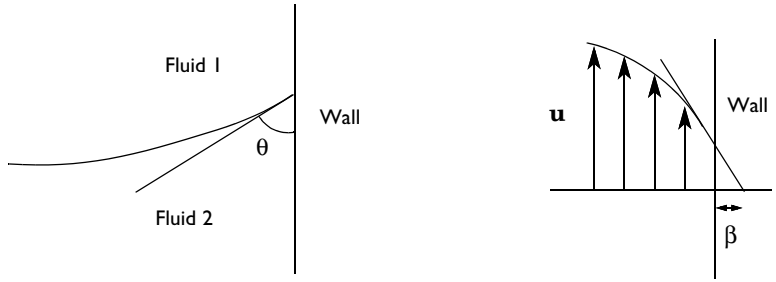


Figure 4-1: Definition of the contact angle θ *at interface/wall contact points (left) and an illustration of the slip length* β *(right).*

SETTINGS

The **Label** is the default multiphysics coupling feature name.

The default **Name** (for the first **Wetted Wall** multiphysics coupling feature in the model) is `ww1`.

BOUNDARY SELECTION

When nodes are added from the context menu, select **All boundaries** (the default) or select **Manual** from the **Selection** list to choose specific boundaries.

COUPLED INTERFACES

This section controls which individual interfaces are coupled by the current coupling feature. If a physics interface is deleted and then added to the model again, then in order to reestablish the coupling, you need to choose the correct physics interface again from the **Fluid flow** or **Moving interfaces** lists.

WALL MOVEMENT

This section contains controls to describe the wall movement relative to the lab (or spatial) frame.

The **Translational velocity** setting controls the translational wall velocity, $\mathbf{u_{tr}}$. The list is per default set to **Automatic from frame**. The physics automatically detects if the spatial frame moves. This can for example happen if an ALE interface is present in the model component. If there is no movement $\mathbf{u_{tr}} = \mathbf{0}$. If the frame moves, $\mathbf{u_{tr}}$ becomes equal to the frame movement.

Select **Manual** from **Translational velocity** selection list in order to manually prescribe **Velocity of moving wall**, $\mathbf{u}_{\mathbf{tr}}$. This can for example be used to model an oscillating wall where the magnitude of the oscillations are very small compared to the rest of the model. Specifying translational velocity manually does not automatically cause the associated wall to move. An additional Moving Mesh interface needs to be added to physically track the wall movement in the spatial reference frame.

Translational velocity can also be set to **Zero (Fixed wall)** to force $\mathbf{u}_{\mathbf{tr}} = \mathbf{0}$. This is typically used in problems where the mesh is deforming or rotating, but we want the boundary to keep zero velocity. For example, in fixed walls tangential to a **Rotating Domain**.

WETTED WALL

When using **Navier Slip**, the **Slip Length** setting is per default set to **Factor of minimum element length**. The slip length β is then defined as $\beta = f_{\mathrm{h}} h_{\mathrm{min}}$, where h_{min} is the smallest element side (corresponds to the element size in the wall normal direction for boundary layer elements) and f_{h} is a user input. Select **User defined** from **Slip Length** selection list in order to manually prescribe β (SI unit: m).

If the fluid physics interface includes porous domains, check **Use porous slip wall treatment** to use the porous slip wall treatment to provide tangential stresses and the slip velocity on boundaries adjacent to porous domains. If **Use porous slip wall treatment** is not checked, the condition selected in **Wall condition** is used for porous boundaries.

CONTACT ANGLE

Select an option from the **Specify contact angle list** — **Directly** (the default) or **Through Young's equation**. For **Directly** enter a **Contact angle** θ_w (SI unit: rad). The default is $\pi/2$ radians. For **Through Young's equation** enter values or expressions for **Phase 1-Solid surface energy density** γ_{s1} (SI unit: $\mathrm{J/m^2}$) and **Phase 2-Solid surface energy density** γ_{s2} (SI unit: $\mathrm{J/m^2}$).

Theory for the Level Set and Phase Field Interfaces

The Interior Wetted Wall Coupling Feature

The **Interior Wetted Wall**, multiphysics coupling boundary feature can only be applied on interior boundaries.

It is similar to The Wetted Wall Coupling Feature available on exterior boundaries of the **Laminar Two-Phase Flow, Level Set** ( ) multiphysics interface, except that it applies on both sides of an interior boundary. It is an exclusive feature which overrides the **Interior Wall** feature in the Laminar interface as well as the **Thin Barrier** feature in the Level Set interface. It is available for laminar flow and turbulent flow with wall functions or automatic wall treatment.

The **Interior Wetted Wall** coupling feature allows discontinuities (velocity, pressure, level set variable) across the boundary and can be used to avoid meshing thin structures in contact with the fluid-fluid interface. When this boundary condition is used, the fluid-fluid interface can move along the wall.

For laminar flow, this boundary condition enforces the no-penetration condition $\mathbf{u} \cdot \mathbf{n}_{\text{wall}} = 0$ on both sides of the wall, and adds a tangential stress on the form

$$\mathbf{K}_{\text{nt}} = -\frac{\mu}{\beta}\mathbf{u}$$

where $\mathbf{K}_{\text{nt}} = \mathbf{K}_{\text{n}} - (\mathbf{K}_{\text{n}} \cdot \mathbf{n}_{\text{wall}})\mathbf{n}_{\text{wall}}$, $\mathbf{K}_{\text{n}} = \mathbf{K}\mathbf{n}_{\text{wall}}$, and $\mathbf{K}$ is the viscous stress tensor. β is the slip length. For numerical calculations, a suitable choice is $\beta = h$, where h is the mesh element size.

If the surface tension force is included in the momentum equation, the **Interior Wetted Wall** boundary condition also adds the following boundary force on both sides of the walls to enforce the contact angle:

$$\mathbf{F}_{\theta} = \sigma\delta(\mathbf{n}_{\text{wall}} \cdot \mathbf{n} - \cos\theta_{\text{w}})\mathbf{n}$$

Note that the contact angle is not enforced on boundaries adjacent to porous domains. For more information, see The Wetted Wall Coupling Feature.

SETTINGS

The **Label** is the default multiphysics coupling feature name.

The default **Name** (for the first **Interior Wetted Wall** multiphysics coupling feature in the model) is `iww1`.

COUPLED INTERFACES

This section controls which individual interfaces are coupled by the current coupling feature. If a physics interface is deleted and then added to the model again, then in order to reestablish the coupling, you need to choose the correct physics interface again from the **Fluid flow** or **Moving interfaces** lists.

WALL MOVEMENT

This section contains controls to describe the wall movement relative to the lab (or spatial) frame.

The **Translational velocity** setting controls the translational wall velocity, $\mathbf{u_{tr}}$. The list is per default set to **Automatic from frame**. The physics automatically detects if the spatial frame moves. This can for example happen if an ALE interface is present in the model component. If there is no movement $\mathbf{u_{tr}} = \mathbf{0}$. If the frame moves, $\mathbf{u_{tr}}$ becomes equal to the frame movement.

Select **Manual** from **Translational velocity** selection list in order to manually prescribe **Velocity of moving wall**, $\mathbf{u_{tr}}$. This can for example be used to model an oscillating wall where the magnitude of the oscillations are very small compared to the rest of the model. Specifying translational velocity manually does not automatically cause the associated wall to move. An additional Moving Mesh interface needs to be added to physically track the wall movement in the spatial reference frame.

BOUNDARY SELECTION

When nodes are added from the context menu, select **All boundaries** (the default) or select **Manual** from the **Selection** list to choose specific boundaries.

WETTED WALL

When using **Navier Slip**, the **Slip Length** setting is per default set to **Factor of minimum element length**. The slip length β is then defined as $\beta = f_h h_{min}$, where h_{min} is the smallest element side (corresponds to the element size in the wall normal direction for boundary layer elements) and f_h is a user input. Select **User defined** from **Slip Length** selection list in order to manually prescribe β (SI unit: m).

If the fluid physics interface includes porous domains, check **Use porous slip wall treatment** to use the porous slip wall treatment to provide tangential stresses and the slip velocity on boundaries adjacent to porous domains. If **Use porous slip wall treatment** is not checked, the condition selected in **Wall condition** is used for porous boundaries.

CONTACT ANGLE

Select an option from the **Specify contact angle list** — **Directly** (the default) or **Through Young's equation**. For **Directly** enter a **Contact angle** θ_w (SI unit: rad). The default is $\pi/2$ radians. For **Through Young's equation** enter values or expressions for **Phase 1-Solid**

surface energy density γ_{s1} (SI unit: J/m^2) and **Phase 2-Solid surface energy density** γ_{s2} (SI unit: J/m^2).

	The Wetted Wall Coupling Feature

The Laminar Two-Phase Flow, Phase Field Interface

The **Laminar Two-Phase Flow, Phase Field** interface ( ) found under the **Multiphase Flow** > **Two-Phase Flow, Phase Field** branch ( ), is a multiphysics interface designed to track the interface between two immiscible fluids. The flow is assumed to be laminar, that is, to be of low to moderate Reynolds number. The fluids can be incompressible or compressible.

When adding the **Laminar Two-Phase Flow, Phase Field** multiphysics interface, a **Laminar Flow** and a **Phase Field in Fluids** interface are added to the Model Builder. In addition, a multiphysics coupling feature, The Two-Phase Flow, Phase Field Coupling Feature, is added automatically under the **Multiphysics** node. Note that unlike the Two-Phase Flow, Level Set interfaces, the wetted wall feature here is not implemented as a separate multiphase coupling boundary feature but as a default **Wetted Wall** feature in the **Phase Field in Fluids** interface.

	Wetted Wall

Simulations using the Laminar Two-Phase Flow, Phase Field interface are always time-dependent since the position of an interface almost always depends on its history.

INTERFACE PROPERTIES

Discretization

By default the fluid flow discretization is set to **P1+P1**, and the phase field discretization is set to **Linear**. This combination provides improved conservation of the integral of the phase field variable when using the nonconservative form of the phase field equations.

	Theory for the Two-Phase Flow Interfaces

The Two-Phase Flow, Phase Field Coupling Feature

The **Laminar Two-Phase Flow, Phase Field** ( ) and **Turbulent Two-Phase Flow, Phase Field** ( ) interfaces contain a multiphysics coupling feature, **Two-Phase Flow, Phase Field**, which is added automatically.

The **Two-Phase Flow, Phase Field** multiphysics coupling feature defines the density and dynamic viscosity of the fluid used in the **Laminar Flow** interfaces, and it defines the surface tension on the interface in form of a volume force used in the momentum equation. It also enables the **Phase Field in Fluids** interface to use the velocity field calculated from the **Laminar Flow**interface to transport the interface.

SETTINGS

The **Label** is the default multiphysics coupling feature name.

The **Name** is used primarily as a scope prefix for variables defined by the coupling node. Refer to such variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different coupling nodes or physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first multiphysics coupling feature **Two-Phase Flow, Phase Field** in the model) is `tpf1`.

DOMAIN SELECTION

When nodes are added from the context menu, you can select **All domains** (the default) or select **Manual** from the **Selection** list to choose specific domains.

COUPLED INTERFACES

This section controls which individual interfaces are coupled by the current coupling feature. If a physics interface is deleted and then added to the model again, then in order to reestablish the coupling, you need to choose the correct physics interface again from the **Fluid flow** or **Moving interfaces** lists.

MODEL INPUTS

Fluid properties of each phase, such as density, viscosity, or the surface tension coefficient, can be defined through user inputs, variables, or by selecting a material. For the latter option, additional inputs, for example temperature or pressure, may be required to define these properties.

Temperature

By default, the **Temperature** model input is set to **Common model input**, and the temperature is controlled from Default Model Inputs under **Global Definitions** or by a locally defined Model Input. If a Heat Transfer interface is included in the component, it controls the temperature **Common model input**. Alternatively, the temperature field can be selected from another physics interface. All physics interfaces have their own tags (**Name**). For example, if a Heat Transfer in Fluids interface is included in the component, the **Temperature (ht)** option is available for T.

You can also select **User defined** from the **Temperature** model input in order to manually prescribe T.

Absolute Pressure

This input appears when a material requires the absolute pressure as a model input. The default **Absolute pressure** p_A is $p+p_{\mathrm{ref}}$, where p is the dependent pressure variable from the Navier–Stokes or RANS equations, and p_{ref} is from the user input defined at the fluid flow physics interface level.

The **Absolute pressure** field can be edited by clicking **Make All Model Inputs Editable** ( ) and entering the desired value in the input field.

	Model Inputs and Multiphysics Couplings in the *COMSOL Multiphysics Reference Manual*

MATERIAL PROPERTIES

The effective density and dynamic viscosity can either be **Locally defined** or picked up from a Multiphase Material. When the properties are defined locally, provide the properties for each phase in the respective fluid properties section, and the averaging method in the advanced settings section. If a multiphase material is used, these settings are controlled from the material. Using a multiphase material is advantageous for models coupling two-phase flow with other physics interfaces, such as Heat Transfer in Fluids or Electrostatics. In such cases, the multiphase material can ensure that the effective material properties for these physics interfaces are averaged using the volume fraction from the Phase Field in Fluids physics interface.

Click the **Go to Material** button ( ) to move to the selected material node. Click the **Add Multiphase Material** button ( ) to add a multiphase material with two phases. The added material then becomes the one selected in the **Multiphase Material** list.

	Multiphase Material in the *COMSOL Multiphysics Reference Manual*

	• *Separation Through Electrocoalescence*: Application Library path **Microfluidics_Module/Two-Phase_Flow/electrocoalescence**

FLUID PROPERTIES

A **Fluid Properties** section will be available per phase if the **Material Properties** are set to **Locally defined**. Use the corresponding section to specify the properties of the two fluids. The fluids are denoted **Fluid 1** and **Fluid 2**, respectively.

To specify the properties of **Fluid 1** from a material, select the appropriate material in the **Fluid 1** list. Also make sure that the **Density of fluid 1** ρ_1 and **Dynamic viscosity of fluid 1** μ_1 are both set to **From Material**.

The density in a material can depend on temperature and/or pressure and these dependencies are automatically replaced by p_{ref} and T_{ref} for incompressible flows (as specified by the **Compressibility** setting of the fluid flow interface).

The non-Newtonian Power law, Carreau, Bingham–Papanastasiou, Herschel–Bulkley–Papanastasiou, and Casson–Papanastasiou models can alternatively be used to specify the dynamic viscosities of the two fluids.

To instead apply a variable or expression for the density or dynamic viscosity for Fluid A, select **User defined** in the **Density of fluid 1** ρ_1 or the **Dynamic viscosity of fluid 1** μ_1 list and enter the expression in the corresponding text field.

Similarly, the properties of **Fluid 2** can be specified. The default material is set to **None**.

⚠	Care should be taken when using the **Domain Material** setting for the material properties for Fluid 1 and Fluid 2. The material properties are obtained from the domain irrespective of the location of the interface. If two different materials are selected in domains 1 and 2, with the phase boundary initially coincident with the domain boundary, the model has convergence issues once the phase boundary moves away from the domain boundary. This is because a density discontinuity and a viscosity discontinuity occurs at the boundary separating the two fluids. For this reason, selecting the material directly is recommended when setting the material properties for Fluid 1 and Fluid 2.

The fluid defined as Fluid 1 affects the wetting characteristics on wetted walls. See the Wetted Wall node for details.

ADVANCED SETTINGS

f the **Material Properties** are set to **Locally defined**, you can specify the averaging method for density and dynamic viscosity in this section. Select the method used for **Density averaging** and **Viscosity averaging**. The default method for both settings is **Volume average**. In addition to the default method, **Density averaging** can be set to **Heaviside function** or **Harmonic volume average**, while **Viscosity averaging** can be set to **Heaviside function**, **Harmonic volume average**, **Mass average**, or **Harmonic mass average**. When a **Heaviside function** is used, enter a value for the corresponding mixing parameter, l_ρ or l_μ.

When the surface tension force is included in the momentum equation, you can select the **Shift surface tension force to the heaviest phase** checkbox. This can prevent significant spurious oscillations in the velocity field for the lighter phase in cases with a large difference in density between the two phases. The amount of shifting is controlled by the **Smoothing factor** $d_{s,Fst}$ (default 0.1). The surface tension force is then multiplied by

$$f_s = \frac{2}{(\rho_1 + \rho_2)}\left(\rho_1 H\left(\frac{V_{f,1} - 0{,}5}{d_{s,Fst}}\right) + \rho_2 H\left(\frac{V_{f,2} - 0{,}5}{d_{s,Fst}}\right)\right) \tag{4-2}$$

Shift surface tension force to the heaviest phase works better when combined with **Heaviside function** for the averaging of density and viscosity.

SURFACE TENSION

Select the **Include surface tension force in momentum equation** checkbox to include the surface tension force in the momentum equation. If the surface tension force is included, select **Include surface tension gradient effects in surface tension force** to account for the Marangoni effect due to gradients in the surface tension coefficient.

Select a **Surface tension coefficient** σ (SI unit: N/m):

- To use a predefined expression, select **Library coefficient, liquid/gas interface** or **Library coefficient, liquid/liquid interface**. Then select an option from the list that displays below (for example, **Water/Air** or **Glycerol/Air**). The predefined correlations are based on the data in Ref. 7, Ref. 8, and Ref. 9.
- For **User defined**, enter a value or expression for the surface tension coefficient σ (SI unit: N/m).

Theory for the Level Set and Phase Field Interfaces

Domain, Boundary, Point, and Pair Nodes for the Laminar Flow, Two-Phase, Level Set and Phase Field Interfaces

The Two-Phase Flow, Level Set and Phase Field interfaces are multiphysics interfaces combining Laminar Flow or Turbulent Flow interfaces together with Level Set or Phase Field in Fluids interfaces.

LAMINAR FLOW

The available physics features for the Laminar Flow interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

LEVEL SET

The available physics features for the Level Set interface are listed in the section Domain, Boundary, and Pair Nodes for the Level Set Interface.

PHASE FIELD IN FLUIDS

The available physics features for the Phase Field in Fluids interface are listed in the section Domain, Boundary, and Pair Nodes for the Phase Field in Fluids Interface.

All domain, boundary, point, and pair nodes are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or by right-clicking to access the context menu (all users).

The Laminar Three-Phase Flow, Phase Field Interface

This section includes the following topics:

- The Laminar Three-Phase Flow, Phase Field Interface
- The Three-Phase Flow, Phase Field Coupling Feature
- Domain, Boundary, Point, and Pair Nodes for the Laminar Three-Phase Flow, Phase Field Interface

	Mathematics, Moving Interfaces

The Laminar Three-Phase Flow, Phase Field Interface

The **Laminar Three-Phase Flow, Phase Field** interface ( ), found under the **Multiphase Flow** > **Three-Phase Flow, Phase Field** branch ( ), is a multiphysics interface designed to track the interfaces between three immiscible and incompressible fluids. The flow is assumed to be laminar; that is, a flow characterized by a low-to-moderate Reynolds number. The density of each fluid is assumed to be constant, but the there is no restriction on the density differences between the separate fluids.

When adding the **Laminar Three-Phase Flow, Phase Field** multiphysics interface, a **Laminar Flow** and a **Ternary Phase Field** interface are added to the Model Builder. In addition the **Multiphysics** node, including the multiphysics coupling feature **Three-Phase Flow, Phase Field** is added.

	The Multiphysics Branch in the *COMSOL Multiphysics Reference Manual*.

Simulations using the Laminar Three-Phase Flow, Phase Field interface are always time-dependent since the position of an interface almost always depends on its history.

The Three-Phase Flow, Phase Field Coupling Feature

Use the **Three-Phase Flow, Phase Field** ( ) multiphysics coupling to simulate the flow of a three immiscible fluids while explicitly tracking the interface separating each pair of the fluids.

The Three-Phase Flow interface solves Navier–Stokes equations for the conservation of momentum, and a continuity equation for the conservation of mass. The positions of the interfaces separating the fluid phases are tracked by solving four additional transport equations: two equations governing phase field variables and two equations for the corresponding generalized chemical potentials. The movement of the fluid-fluid interfaces is determined by minimization of free energy.

SETTINGS

The **Label** is the default multiphysics coupling feature name.

The **Name** is used primarily as a scope prefix for variables defined by the coupling node. Refer to such variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different coupling nodes or physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first multiphysics coupling feature in the model) is `tfpf1`.

DOMAIN SELECTION

When nodes are added from the context menu, you can select **Manual** (the default) from the **Selection** list to choose specific domains to define the three-phase flow, or select **All domains** as needed.

MODEL INPUTS

Fluid properties of each phase, such as density and viscosity, can be defined through user inputs, variables, or by selecting a material. For the latter option, additional inputs, for example temperature or pressure, may be required to define these properties.

Temperature

By default, the **Temperature** model input is set to **Common model input**, and the temperature is controlled from Default Model Inputs under **Global Definitions** or by a locally defined Model Input. If a Heat Transfer interface is included in the component, it controls the temperature **Common model input**. Alternatively, the temperature field can be selected from another physics interface. All physics interfaces have their own

tags (**Name**). For example, if a Heat Transfer in Fluids interface is included in the component, the **Temperature (ht)** option is available for T.

You can also select **User defined** from the **Temperature** model input in order to manually prescribe T.

Absolute Pressure

This input appears when a material requires the absolute pressure as a model input. The default **Absolute pressure** p_A is $p + p_{\text{ref}}$, where p is the dependent pressure variable from the Navier–Stokes equations, and p_{ref} is from the user input defined at the fluid flow physics interface level.

The **Absolute pressure** field can be edited by clicking **Make All Model Inputs Editable** ( ) and entering the desired value in the input field.

	Model Inputs and Multiphysics Couplings in the *COMSOL Multiphysics Reference Manual*

MATERIAL PROPERTIES

The effective density and dynamic viscosity can either be **Locally defined** or picked up from a Multiphase Material. When the properties are defined locally, provide the properties for each phase in the respective fluid properties section, and the averaging method in the advanced settings section. If a multiphase material is used, these settings are controlled from the material. Using a multiphase material is advantageous for models coupling two-phase flow with other physics interfaces, such as Heat Transfer in Fluids or Electrostatics. In such cases, the multiphase material can ensure that the effective material properties for these physics interfaces are averaged using the volume fraction from the Ternary Phase Field physics interface.

Click the **Go to Material** button ( ) to move to the selected material node. Click the **Add Multiphase Material** button ( ) to add a multiphase material with three phases. The added material then becomes the one selected in the **Multiphase Material** list.

	Multiphase Material in the *COMSOL Multiphysics Reference Manual*

FLUID PROPERTIES

A **Fluid Properties** section will be available per phase if the **Material Properties** are set to **Locally defined**. Use the corresponding section to specify the properties of all three fluids. The fluids are denoted **Fluid A**, **Fluid B**, and **Fluid C**, respectively.

To specify the properties of **Fluid A** from a material, select the appropriate material in the **Fluid A** list. Also make sure that the **Density of fluid A** ρ_A and **Dynamic viscosity of fluid A** μ_A are both set to **From material**.

The density in a material can depend on temperature and/or pressure and these dependencies are automatically replaced by p_{ref} and T_{ref} for incompressible flows (as specified by the **Compressibility** setting of the laminar flow interface).

The non-Newtonian Power law, Carreau, Bingham–Papanastasiou, Herschel–Bulkley–Papanastasiou, and Casson–Papanastasiou models can alternatively be used to specify the dynamic viscosities of the three fluids.

To instead apply a variable or expression for the density or dynamic viscosity for Fluid A, select **User defined** in the **Density of fluid A** ρ_A or the **Dynamic viscosity of fluid A** μ_A list and enter the expression in the corresponding text field.

COUPLED INTERFACES

This section controls which individual interfaces are coupled by the current coupling feature. If a physics interface is deleted and then added to the model again, then in order to reestablish the coupling, you need to choose the correct physics interface again from the **Fluid flow** or **Moving interfaces** lists.

- Theory for the Level Set and Phase Field Interfaces

Domain, Boundary, Point, and Pair Nodes for the Laminar Three-Phase Flow, Phase Field Interface

The Laminar Three-Phase Flow, Phase Field Interface is a multiphysics interface combining The Laminar Flow Interface and The Ternary Phase Field Interface.

LAMINAR FLOW

The available physics features for The Laminar Flow Interface are listed in Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TERNARY PHASE-FIELD

The available physics features for The Ternary Phase Field Interface are listed in Domain, Boundary, and Pair Nodes for the Ternary Phase Field Interface.

All domain, boundary, point, and pair nodes are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or by right-clicking to access the context menu (all users).

The Laminar Two-Phase Flow, Moving Mesh Interface

The **Laminar Two-Phase Flow, Moving Mesh** interface ( ), found under the **Multiphase Flow** > **Two-Phase Flow, Moving Mesh** branch ( ), is a multiphysics interface designed to model laminar two–phase flow of immiscible fluids separated by a moving interface. The velocity field, pressure, and mesh deformation are solved for, and the location of the interface is tracked by the deformed mesh.

When adding the **Laminar Two-Phase Flow, Moving Mesh** multiphysics interface, a **Laminar Flow** interface is added to the component, and a **Moving Mesh** interface with a **Deforming Domain** feature is added under the **Definitions** node. The **Laminar Flow** interface adds the Navier–Stokes equations and provides a way of defining the properties of the fluids. For each of the fluids the density and viscosity must be specified (these are typically taken from the corresponding materials, but can be user defined).

Simulations using the **Laminar Two-Phase Flow, Moving Mesh** interface are always time-dependent since the position of an interface is almost always dependent of its history. There are additional boundary conditions to describe how the fluid-fluid interface moves from the **Laminar Flow** context menu under the option **Fluid Interface Features**:

- Fluid-Fluid Interface
- Free Surface
- Contact Angle (as a subfeature to the two conditions above)

	In previous versions of COMSOL Multiphysics (prior to version 5.4), a specific physics interface called **Laminar Two-Phase Flow, Moving Mesh (tpfmm)** was added to the **Model Builder**. Now, a predefined multiphysics coupling approach is used, improving the flexibility and design options for your modeling. For specific details, see The Multiphysics Branch and Multiphysics Modeling Workflow in the *COMSOL Multiphysics Reference Manual*.

Select Laminar Flow Properties

For a full list of available properties, see The Laminar Flow Interface.

PHYSICAL MODEL

This physics interface deforms the mesh within the domains on either side of the two fluid interfaces to track its movement.

The **Compressibility** defaults to **Incompressible flow** to use the incompressible (constant density) formulation of the Navier–Stokes equations. Select **Compressible flow (Ma<0.3)** to use the compressible formulation.

If flow is occurring at very low Reynolds numbers, the inertial term in the Navier–Stokes equations can be neglected and the linear Stokes equations can be solved on the domain. This flow type is referred to as *creeping flow* or *Stokes flow* and can occur in microfluidics and MEMS devices, where the flow length scales are very small. To make this approximation select the **Neglect inertial term (Stokes flow)** checkbox, which significantly improves the solver speed.

Enter a **Reference pressure level** p_{ref} (SI unit: Pa). The default value is `1[atm]`.

DEPENDENT VARIABLES

The dependent variables (field variables) are for the **Velocity field** and **Pressure**. The names can be changed in the corresponding fields, but the names of fields and dependent variables must be unique within a model.

The following models are found at this Application Library path **Microfluidics_Module/Two-Phase_Flow/<filename>**

- *Drug Delivery System*: **viscous_catenary**
- *Jet Instability — Moving Mesh*: **jet_instability**
- *Electrowetting Lens*: **electrowetting_lens**
- *Viscous Catenary*: **viscous_catenary**

Deforming Domain

When the **Laminar Two-Phase Flow, Moving Mesh** multiphysics interface is added using the **Model Wizard**, a **Deforming Domain** node is added automatically in the **Model Builder** under the **Definitions** > **Moving Mesh** node. This node serves to represent domains and boundaries where the mesh can deform. By default, the selection is all domains. Under

the **Deforming Domain**, you can also choose the **Mesh smoothing type**, by default set to **Yeoh** with a default **Stiffening factor** of 10. More information of the smoothing type can be found in the Deforming Domain chapter in the *COMSOL Multiphysics Reference Manual*.

By default, the mesh is fixed at all external boundaries of the geometry. Use the Symmetry/Roller node to select the external boundaries, where the fluid-fluid interface can slide along the boundary. You can also add other types of boundary conditions for the mesh motion, for details see Moving Mesh Features in the *COMSOL Multiphysics Reference Manual*.

Fluid-Fluid Interface

The **Fluid-Fluid Interface** node defines the initial position of a fluid-fluid interface and includes equations to track the evolution of the interface. The Contact Angle subnode is added by default, and is also available from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu.

MODEL INPUT

Enter a value for the **Temperature** T (SI unit: K). This option is only necessary when the surface tension coefficient comes from a library of coefficients, as explained below.

SURFACE TENSION

Select the **Include surface tension force in momentum equation** checkbox to include the surface tension force in the momentum equation.

The **Surface tension coefficient** σ (SI unit: N/m) can be **User defined**, or select **Library coefficient, liquid/gas interface** (default) or **Library coefficient, liquid/liquid interface**.

- For **Library coefficient, liquid/gas interface** select an option from the list — **Water/Air** (default), **Acetone/Air**, **Acetic acid/Air**, **Ethanol/Air**, **Ethylene glycol/Ethylene glycol vapor**, **Diethyl ether/Air**, **Glycerol/Air**, **Heptane/Nitrogen**, **Mercury/Mercury vapor**, or **Toluene/Air**.
- For **Library coefficient, liquid/liquid interface** select an option from the list — **Benzene/Water, 20°C**, **Corn oil/Water, 20°C**, **Ether/Water, 20°C**, **Hexane/Water, 20°C**, **Mercury/Water, 20°C**, or **Olive oil/Water, 20°C**.

The predefined correlations are based on the data in Ref. 5, Ref. 6, and Ref. 7.

MASS FLUX

The mass flux setting specifies the mass transfer across the boundary, due to processes such as boiling. The default **Mass Flux** M_f (SI unit: kg/(m^2·s)) is **User defined**, with a value of 0.

NORMAL DIRECTION

The normal direction on the selected boundaries can be reversed by selecting **Reverse normal direction**. The direction is indicated by a red arrow in the Graphics window.

	The **Fluid-Fluid Interface** feature imposes a mesh deformation in the normal direction. On adjacent boundaries, the mesh displacement parallel to those boundaries cannot be fixed if the contact point is moving. In this case a Mesh Slip, Symmetry/Roller, Prescribed Normal Mesh Displacement, or Prescribed Normal Mesh Velocity boundary condition under **Definitions>Moving Mesh** should be selected. A Mesh Slip condition is automatically used on boundaries that are adjacent to the Fluid-Fluid Interface and dot not have a prescribed Moving Mesh boundary condition.

	If a **Fluid-Fluid Interface** feature is in contact with a solid boundary, the movement of the contact point is not compatible with the no slip condition. For laminar flow the Wall boundary condition with the Navier Slip option should be selected.

Free Surface

The **Free Surface** node defines the initial position of an external fluid interface - that is, an interface in which the viscosity in the fluid outside the domain can be neglected. By applying this feature the motion of the two-phase interface can be tracked. In the tangential direction the free surface motion is governed by the fluid motion in combination with the surface tension of the fluid-fluid interface.

The Free Surface node can only be applied to outer boundaries of a **Deforming Domain** that do not have any boundary condition assigned under **Moving Mesh**.

To control the attachment angle between the free surface and adjacent walls, a Contact Angle subnode is by default added under the **Free Surface** node. A different contact

angle subnode can be added from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu.

MODEL INPUT

Enter a value for the **Temperature** T (SI unit: K). This option is only necessary when the surface tension coefficient comes from a library of coefficients, as explained below.

FREE SURFACE

Enter an **External pressure** p_{ext} (SI unit: Pa).

SURFACE TENSION

Select the **Include surface tension force in momentum equation** checkbox to include the surface tension force in the momentum equation.

The default **Surface tension coefficient** σ (SI unit: N/m) can be **User defined**, or select **Library coefficient, liquid/gas interface** (default) or **Library coefficient, liquid/liquid interface**.

- For **Library coefficient, liquid/gas interface** select an option from the list — **Water/Air** (default), **Acetone/Air**, **Acetic acid/Air**, **Ethanol/Air**, **Ethylene glycol/Ethylene glycol vapor**, **Diethyl ether/Air**, **Glycerol/Air**, **Heptane/Nitrogen**, **Mercury/Mercury vapor**, or **Toluene/Air**.
- For **Library coefficient, liquid/liquid interface** select an option from the list — **Benzene/Water, 20°C**, **Corn oil/Water, 20°C**, **Ether/Water, 20°C**, **Hexane/Water, 20°C**, **Mercury/Water, 20°C**, or **Olive oil/Water, 20°C**.

The predefined correlations are based on the data in Ref. 5, Ref. 6, and Ref. 7.

MASS FLUX

The mass flux setting specifies the mass transfer across the boundary, due to processes such as boiling. The default **Mass Flux** M_f (SI unit: kg/(m^2·s)) is **User defined**, with a value of 0.

	The **Free Surface** feature imposes a mesh deformation in the normal direction. On adjacent boundaries, the mesh displacement parallel to those boundaries cannot be fixed if the contact point is moving. In this case a Mesh Slip, Symmetry/Roller, Prescribed Normal Mesh Displacement, or Prescribed Normal Mesh Velocity boundary condition under **Definitions>Moving Mesh** should be selected. A Mesh Slip condition is automatically used on boundaries that are adjacent to the Free Surface and dot not have a prescribed Moving Mesh boundary condition.

	If a **Free Surface** feature is in contact with a solid boundary, the movement of the contact point is not compatible with the no slip condition. For laminar flow the **Wall** boundary condition with the **Navier Slip** option should be selected.

Contact Angle

The **Contact Angle** subnode is available from the context menu (right-click the Fluid-Fluid Interface or Free Surface parent node) or from the **Physics** toolbar, **Attributes** menu. The condition applies forces on the wall that balance the surface tension for the prescribed contact angle. Note that the contact angle can only be enforced when the surface tension force is included in the momentum equation in the parent feature.

For laminar flow with moving mesh, the **Contact Angle** node should be used on edges or points where a Wall feature with the **Navier Slip** option is prescribed adjacent to the free surface. In this case, the **Navier Slip** option is required for the contact line to move along the wall.

The representation of the contact angle is dependent on the mesh resolution in the region where the fluid-fluid interface attaches to the wall. If, during the simulation, the contact angle is found to fluctuate around a given value, this indicates that the resolution needs to be improved. This can for example be achieved by adding more mesh boundary layers on the wall.

CONTACT ANGLE

Select an option from the **Specify contact angle list** — **Directly** (the default) or **Through Young's equation**.

- For **Directly** enter a **Contact angle** θ_w (SI unit: rad). The default is $\pi/2$ radians.
- For **Through Young's equation** enter values or expressions for **Phase 1-Solid surface energy density** γ_{s1} (SI unit: J/m^2) and **Phase 2-Solid surface energy density** γ_{s2} (SI unit: J/m^2).

NORMAL WALL VELOCITY

Select whether to **Constrain the wall-normal velocity**. This ensures that the fluid velocity normal to the wall on the contact edge or point is exactly the desired value. This can be helpful when the adjacent wall uses a Nitsche Constraints and the no-penetration condition is satisfied in an integral sense rather than pointwise. Moreover, constraining the wall-normal velocity simplifies the equilibrium of forces in the wall-normal direction. This setting should not be selected when the adjacent boundary has an unknown velocity.

	The contact angle θ_w is defined between the fluid-fluid interface and the surface of the wall adjacent to phase 1.

!	The moving mesh boundary condition must be compatible with the motion of the wall for the problem to have a valid solution.

Theory for the Level Set and Phase Field Interfaces

The Two-Phase Flow, Level Set and Phase Field interfaces can be used to model the flow of two different, immiscible fluids, where the exact position of the interface between the two fluids is of interest. The fluid-fluid interface is tracked using an auxiliary function on a fixed mesh. These methods account for differences in the two fluids' densities and viscosities and include the effects of surface tension and gravity.

The Laminar Two-Phase Flow, Level Set and Laminar Two-Phase Flow, Phase Field Interfaces theory is described in this section:

- Level Set and Phase Field Equations
- Conservative and Nonconservative Formulations
- Phase Initialization
- Numerical Stabilization
- References for the Level Set and Phase Field Interfaces

Level Set and Phase Field Equations

By default, the Level Set and Phase Field interfaces use the incompressible formulation of the Navier–Stokes equations:

$$\rho\frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot[-p\mathbf{I} + \mu(\nabla\mathbf{u} + \nabla\mathbf{u}^T)] + \mathbf{F}_g + \mathbf{F}_{st} + \mathbf{F}_{ext} + \mathbf{F} \qquad (4\text{-}3)$$

$$\nabla\cdot\mathbf{u} = 0 \qquad (4\text{-}4)$$

Note that Equation 4-3, and Equation 4-4 are solved in the contained interface, **Laminar Flow** or **Turbulent Flow** interface. Note that the form of the continuity equation, appropriate for high density difference mixtures, differs from the definition in Theory for the Single-Phase Flow Interfaces.

USING THE LEVEL SET METHOD

If the level set method is used to track the interface, it adds the following equation:

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \gamma \nabla \cdot \left(\varepsilon \nabla \phi - \phi(1-\phi) \frac{\nabla \phi}{|\nabla \phi|} \right) \tag{4-5}$$

where γ is the reinitialization parameter (set to 1 by default), and ε is the interface thickness controlling parameter (set proportional to $h_{\max}$ where $h_{\max}$ is the maximum element size in the component). The density is a function of the level set function. Let ρ_1 and ρ_2 be the constant densities of Fluid 1 and Fluid 2, respectively. Here, Fluid 1 corresponds to the domain where $\phi < 0.5$, and Fluid 2 corresponds to the domain where $\phi > 0.5$. When **Density averaging** is set to **Volume average**, the density is defined as,

$$\rho = \rho_1 + (\rho_2 - \rho_1)\phi$$

switching to **Heaviside function**, the density is defined as,

$$\rho = \rho_1 + (\rho_2 - \rho_1)\mathrm{H}\left(\frac{\phi - 0{,}5}{l_\rho}\right)$$

where H is a smooth step function and l_ρ is a mixing parameter defining the size of the transition zone. When the **Harmonic volume average** is selected,

$$\rho = \frac{1}{(1-\phi)/\rho_1 + \phi/\rho_2}$$

Similarly, the dynamic viscosity can be defined by setting **Viscosity averaging** to **Volume average**,

$$\mu = \mu_1 + (\mu_2 - \mu_1)\phi$$

Heaviside function,

$$\mu = \mu_1 + (\mu_2 - \mu_1)\mathrm{H}\left(\frac{\phi - 0{,}5}{l_\mu}\right)$$

Harmonic volume average,

$$\mu = \frac{1}{(1-\phi)/\mu_1 + \phi/\mu_2}$$

Mass average,

$$\mu = \frac{\rho_1(1-\phi)\mu_1 + \rho_2\phi\mu_2}{\rho}$$

or **Harmonic mass average**,

$$\mu = \frac{\rho}{\rho_1(1-\phi)/\mu_1 + \rho_2\phi/\mu_2}$$

where μ_1 and μ_2 are the dynamic viscosities of Fluid 1 and Fluid 2, respectively. For inelastic non-Newtonian fluids, $\mu_{1,2}$ is replaced by $\mu_{\text{app}1,2}$ in the previous expressions. Further details of the theory for the level set method are in Ref. 1.

USING THE PHASE FIELD METHOD

If the phase field method is used to track the interface, it adds the following equations:

$$\frac{\partial\phi}{\partial t} + \mathbf{u}\cdot\nabla\phi = \nabla\cdot\frac{\gamma\lambda}{\varepsilon^2}\nabla\psi \tag{4-6}$$

$$\psi = -\nabla\cdot\varepsilon^2\nabla\phi + (\phi^2-1)\phi + \left(\frac{\varepsilon^2}{\lambda}\right)\frac{\partial f_{\text{ext}}}{\partial\phi} \tag{4-7}$$

where the quantity λ (SI unit: N) is the mixing energy density and ε (SI unit: m) is a capillary width that scales with the thickness of the interface. These two parameters are related to the surface tension coefficient, σ (SI unit: N/m), through the equation

$$\sigma = \frac{2\sqrt{2}}{3}\frac{\lambda}{\varepsilon}$$

and γ is the mobility parameter which is related to ε through $\gamma = \chi\varepsilon^2$ where χ is the mobility tuning parameter (set to 1 by default). The volume fractions of Fluid 1 and Fluid 2 are computed as

$$V_{\text{f},2} = \min(\max([(1+\phi)/2], 0), 1), \qquad V_{\text{f},1} = 1 - V_{\text{f},2}$$

where the `min` and `max` operators are used so that the volume fractions have a lower limit of 0 and an upper limit of 1. Let ρ_1 and ρ_2 be the constant densities of Fluid 1 and Fluid 2, respectively. When **Density averaging** is set to **Volume average**, the density is defined as,

$$\rho = \rho_1 V_{\text{f},1} + \rho_2 V_{\text{f},2}$$

switching to **Heaviside function**, the density is defined as,

$$\rho = \rho_1 + (\rho_2 - \rho_1)\mathrm{H}\left(\frac{V_{\text{f},2} - 0{,}5}{l_\rho}\right)$$

where H is a smooth step function and l_ρ is a mixing parameter defining the size of the transition zone. When the **Harmonic volume average** is selected,

$$\rho = \frac{1}{V_{f,1}/\rho_1 + V_{f,2}/\rho_2}$$

Similarly, the dynamic viscosity can be defined by setting **Viscosity averaging** to **Volume average**,

$$\mu = V_{f,1}\mu_1 + \mu_2 V_{f,2}$$

Heaviside function,

$$\mu = \mu_1 + (\mu_2 - \mu_1)\mathrm{H}\left(\frac{V_{f,2} - 0{,}5}{l_\mu}\right)$$

Harmonic volume average,

$$\mu = \frac{1}{V_{f,1}/\mu_1 + V_{f,2}/\mu_2}$$

Mass average,

$$\mu = \frac{\rho_1 V_{f,1}\mu_1 + \rho_2 V_{f,2}\mu_2}{\rho}$$

or **Harmonic mass average**,

$$\mu = \frac{\rho}{\rho_1 V_{f,1}/\mu_1 + \rho_2 V_{f,2}/\mu_2}$$

where μ_1 and μ_2 are the dynamic viscosities of Fluid 1 and Fluid 2, respectively. For inelastic non-Newtonian fluids, $\mu_{1,2}$ are replaced by $\mu_{\mathrm{app}1,2}$ in the previous expressions.

The mean curvature (SI unit: 1/m) can be computed by entering the following expression:

$$\kappa = 2(1+\phi)(1-\phi)\frac{G}{\sigma}$$

where G is the chemical potential defined as:

$$G = \lambda\left(-\nabla^2\phi + \frac{\phi(\phi^2 - 1)}{\varepsilon^2}\right) + \frac{\partial f}{\partial \phi}$$

Details of the theory for the phase field method are found in Ref. 2.

FORCE TERMS

The four forces on the right-hand side of Equation 4-3 are due to gravity, surface tension, a force due to an external contribution to the free energy (using the phase field method only), and a user-defined volume force.

The Surface Tension Force for the Level Set Method

For the level set method, the surface tension force acting on the interface between the two fluids is:

$$\mathbf{F}_{\mathrm{st}} = \sigma\delta\kappa\mathbf{n} + \delta\nabla_s\sigma$$

where σ is the surface tensions coefficient (SI unit: N/m), $\mathbf{n}$ is the unit normal to the interface, and $\kappa = -\nabla \cdot \mathbf{n}$ is the curvature. δ (SI unit: 1/m) is a Dirac delta function located at the interface. ∇_s is the surface gradient operator

$$\nabla_s = (\mathbf{I} - \mathbf{n}\mathbf{n}^T)\nabla$$

The δ-function is approximated by a smooth function according to

$$\delta = 6|\nabla\phi||\phi(1-\phi)|$$

The Surface Tension Force for the Phase Field Method

The surface tension force for the phase field method is implemented as a body force

$$\mathbf{F}_{\mathrm{st}} = \left(G - \frac{\partial f}{\partial \phi}\right)\nabla\phi$$

where G is the chemical potential (SI unit: J/m^3) defined in The Equations for the Phase Field Method and $\partial f/\partial\phi$ is a user-defined source of free energy. When **Shift surface tension force to the heaviest phase** is selected the surface-tension force is added as,

$$\mathbf{F}_{\mathrm{st}} = \frac{2}{\rho_1 + \rho_2}\left(\rho_1 H\left(\frac{V_{\mathrm{f},1} - 0.5}{d_{s,Fst}}\right) + \rho_2 H\left(\frac{V_{\mathrm{f},2} - 0.5}{d_{s,Fst}}\right)\right)\left(G - \frac{\partial f}{\partial \phi}\right)\nabla\phi$$

where $d_{s,Fst}$ is a smoothing factor. This can be used to avoid unphysical acceleration of a light phase near a phase interface caused by the smearing of the phase interface across a few mesh cells.

If **Include surface tension gradient effects in surface tension force** is selected, extra terms are added to account for the Marangoni effect due to gradients in the surface tension coefficient (see Ref. 6):

$$\mathbf{F}_{\mathrm{st}} = \left(G - \frac{\partial f}{\partial \phi}\right)\nabla\phi + \left(\frac{|\nabla\phi|^2}{2\partial\phi} + \frac{(\phi^2 - 1)^2}{4\varepsilon^2}\right)\nabla\lambda - (\nabla\lambda \cdot \nabla\phi)\nabla\phi$$

The Gravity Force

The gravity force is $\mathbf{F}_g = \rho\mathbf{g}$ where $\mathbf{g}$ is the gravity vector. Add this as a Gravity feature to the fluid domain.

The User-Defined Volume Force

When using a Phase Field interface, a force arising due to a user-defined source of free energy is computed according to:

$$\mathbf{F}_{\mathrm{ext}} = \left(\frac{\partial f}{\partial \phi}\right)\nabla\phi$$

This force is added when a ϕ-derivative of the external free energy has been defined in the External Free Energy section of the Fluid Properties feature.

Conservative and Nonconservative Formulations

When the velocity field is divergence free, you can use either the conservative or the nonconservative formulation of the level set or phase field equation. The conservative form perfectly conserves the mass of each fluid, but the computational time is generally longer.

When the Level Set or Phase Field in Fluids interface are coupled to a fluid flow interface by means of The Two-Phase Flow, Level Set Coupling Feature or The Two-Phase Flow, Phase Field Coupling Feature, improved conservation of the integral of the level set or phase field variable is obtained using the nonconservative form provided that the discretization order of the level set or phase field variable is equal to or lower than the order of the pressure.

Phase Initialization

If the study type Transient with Phase Initialization is used in the model, the level set or phase field variable is automatically initialized. For this study, two study steps are created: Phase Initialization and Time Dependent. The Phase Initialization step solves for the distance to the initial interface, D_{wi}. The Time Dependent step then uses the initial condition for the level set function according to the expression

$$\phi_0 = \frac{1}{1 + e^{D_{\mathrm{wi}}/\varepsilon}}$$

in domains initially filled with Fluid 1 and

$$\phi_0 = \frac{1}{1 + e^{-D_{\mathrm{wi}}/\varepsilon}}$$

in domains initially filled with Fluid 2.

Correspondingly, the phase field method uses the expressions

$$\phi_0 = -\tanh\left(\frac{D_{\mathrm{wi}}}{\sqrt{2}\varepsilon}\right)$$

in Fluid 1 and

$$\phi_0 = \tanh\left(\frac{D_{\mathrm{wi}}}{\sqrt{2}\varepsilon}\right)$$

in Fluid 2. The initial condition for the help variable is $\psi_0 = 0$. These expressions are based on the analytical solution of the steady state solution of Equation 4-5, Equation 4-6, and Equation 4-7 for a straight, nonmoving interface.

!	If the **Phase Initialization** ( ) study step is being used, for the initialization to work it is crucial that there are two **Initial Values** nodes. One of the Initial Values nodes should use **Specify phase: Fluid 1** and the other **Specify phase: Fluid 2**. The initial fluid-fluid interface is then automatically placed on all interior boundaries between both phases. Note that when the value of **Level set variable** or **Phase field variable** is set to **User defined**, arbitrary user defined initial values have to be provided. In this case, the smooth initialization is not used, and a Time Dependent study should be used instead of Time Dependent with Phase Initialization.

	• The Laminar Two-Phase Flow, Level Set and Laminar Two-Phase Flow, Phase Field Interfaces • Studies and Solvers and Time Dependent with Phase Initialization in the *COMSOL Multiphysics Reference Manual*

Numerical Stabilization

Three types of stabilization methods are available for the flow (Navier–Stokes) and interface (level set or phase field) equations. Two are consistent stabilization methods — Streamline diffusion and Crosswind diffusion — and one is inconsistent — Isotropic diffusion.

To display this section, click the **Show More Options** button ( ) and select **Stabilization** from the **Show More Options** dialog.

	• Theory for the Level Set and Phase Field Interfaces • Selection Information in the *COMSOL Multiphysics Reference Manual*

References for the Level Set and Phase Field Interfaces

1. E. Olsson and G. Kreiss, "A Conservative Level Set Method for Two Phase Flow", *J. Comput. Phys.*, vol. 210, pp. 225–246, 2005.

2. P. Yue, J.J. Feng, C. Liu, and J. Shen, "A Diffuse-interface Method for Simulating Two-phase Flows of Complex Fluids", *J. Fluid Mech.*, vol. 515, pp. 293–317, 2004.

3. B. Lafaurie, C. Nardone, R. Scardovelli, S. Zaleski, and G. Zanetti "Modelling Merging and Fragmentation in Multiphase Flows with SURFER.", *J. Comput. Phys.*, vol. 113, no. 1, pp. 134–147, 1994.

4. Y. D. Shikhmurzaev, "The Moving Contact line on a Smooth Solid Surface", *Int. J. Multiph. Flow*, vol. 19, no. 4, pp. 589–610, 1993.

5. J. F. Gerbeau and T. Lelièvre, "Generalized Navier Boundary Condition and Geometric Conservation Law for surface tension", *Comput. Methods Appl. Mech. Eng*, vol. 198, no. 5-8, pp. 644–656, 2009.

6. C. Liu, J. Shen, J. J. Feng, and P. Yue, "Variational Approach in Two-Phase Flows of Complex Fluids: Transport and Induced Elastic Stress", Chapter 11 in *Mathematical Models and Methods in Phase Transitions*, Alan Miranville, ed, Nova Publishers, pp. 259–278, 2005.

7. J. J. Jasper, "The Surface Tension of Pure Liquid Compounds", *J. Phys. Chem. Ref. Data.*, vol. 1, no. 4, pp. 841-1009, 1972.

8. R. C. Weast, ed.,"CRC Handbook of Chemistry and Physics", ed. 69, MIT Press, 1988.

9. A. G. Gaonkar, "Interfacial Tensions of Vegetable Oil/Water Systems: Effect of Oil Purification", *J. Am. Oil Chem. Soc.*, vol. 66, no. 8, pp. 1090-1092, 1989.

Theory for the Three-Phase Flow, Phase Field Interface

The Three-Phase Flow, Phase Field interface can be used to model the flow and interaction of three different, immiscible fluids, when the exact positions of the interfaces separating the fluids are of interest. The fluid-fluid interfaces are tracked using a ternary phase field formulation which account for differences in the fluids' densities and viscosities and include the effects of surface tension.

The Laminar Three-Phase Flow, Phase Field Interface theory is described in the following sections:

- Governing Equations of the Three-Phase Flow, Phase Field Interface
- Reference for the Three-Phase Flow, Phase Field Interface

Governing Equations of the Three-Phase Flow, Phase Field Interface

LAMINAR FLOW EQUATIONS

The Three-Phase Flow, Phase Field interface is used to study the evolution of three immiscible fluid phases denoted by fluid A, fluid B, and fluid C. The interface solves the Navier–Stokes equations governing conservation of momentum and mass. The momentum equations solved correspond to

$$\rho\frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot\left[-p\mathbf{I} + \mu(\nabla\mathbf{u} + \nabla\mathbf{u}^T) - \frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right] + \mathbf{F}_{\mathrm{st}} + \mathbf{F} \qquad (4\text{-}8)$$

where $\mathbf{F}_{\mathrm{st}}$ is the surface tension force. The physics interface assumes that the density of each phase is constant. The density may however vary between the phases. In order to accurately handle systems where density of the phases are significantly different, as well as systems with phases of similar density, the following fully compressible continuity equation is solved by the interface

$$\frac{\partial \log\rho}{\partial t} + \nabla\cdot\mathbf{u} + \mathbf{u}\cdot\nabla\log\rho = 0 \qquad (4\text{-}9)$$

TERNARY PHASE-FIELD EQUATIONS

In order to track the interfaces between three immiscible fluids, a ternary phase field model based on the work of Boyer and co-workers in Ref. 1 is used. The model solves the following Cahn–Hilliard equations

$$\begin{aligned} \frac{\partial \phi_i}{\partial t} + \nabla \cdot (\mathbf{u}\phi_i) &= \nabla \cdot \left(\frac{M_0}{\Sigma_i}\nabla \eta_i\right) \\ \eta_i &= \frac{4\Sigma_T}{\varepsilon}\sum_{j \neq i}\left(\frac{1}{\Sigma_j}\left(\frac{\partial F}{\partial \phi_i} - \frac{\partial F}{\partial \phi_j}\right)\right) - \frac{3}{4}\varepsilon\Sigma_j\nabla^2\phi_i \end{aligned} \tag{4-10}$$

governing the phase field variable, ϕ_i, and a generalized chemical potential, η_i, of each phase $i = A, B, C$. The phase field variables vary between 0 and 1 and are a measure of the concentration of each phase. The phase field variable for phase A is one in instances containing only this phase, and zero where there is no phase A. Since the fluids are immiscible, variations in the phase field variable occur, and define the interface separating two phases. At each point the phase field variables satisfy the following constraint

$$\sum_{i = A, B, C} \phi_i = 1 \tag{4-11}$$

The density of each phase is assumed to be constant which implies that the phase field variable corresponds to the volume fraction of the phase in question. In order to satisfy Equation 4-11, two sets of the equations shown in Equation 4-10 are solved, namely those for phase A and phase B. The phase field variable, and correspondingly the mass fraction, for fluid C is computed from Equation 4-11.

The density and viscosity of the fluid mixture used in Equation 4-3 and 4-4 are defined as:

$$\begin{aligned} \rho &= \rho_A\phi_A + \rho_B\phi_B + \rho_C\phi_C \\ \mu &= \mu_A\phi_A + \mu_B\phi_B + \mu_C\phi_C \end{aligned} \tag{4-12}$$

Free Energy

The free energy of the three phase system is defined as a function of the phase field variables in the manner of:

$$F = \sigma_{AB}\phi_A^2\phi_B^2 + \sigma_{AC}\phi_A^2\phi_C^2 + \sigma_{BC}\phi_B^2\phi_C^2 + \phi_A\phi_B\phi_C(\Sigma_A\phi_A + \Sigma_B\phi_B + \Sigma_C\phi_C) + \Lambda\phi_A^2\phi_B^2\phi_C^2 \tag{4-13}$$

Here the σ_{ij} denotes the surface tension coefficient of the interface separating phase i and j, and the capillary parameters Σ_i are defined for each phase in the manner of:

$$\begin{aligned}\Sigma_A &= \sigma_{AB} + \sigma_{AC} - \sigma_{BC}\\ \Sigma_B &= \sigma_{AB} + \sigma_{BC} - \sigma_{AC}\\ \Sigma_C &= \sigma_{BC} + \sigma_{AC} - \sigma_{AB}\end{aligned} \tag{4-14}$$

Λ in the free energy is a function or parameter specifying the additional free bulk energy of the system. By default Λ is zero. In this case it can be seen that the free energy in Equation 4-13 represents the mixing energy, since only interfaces between two phases (where two phase field variables varies between the limiting values) contributes to the free energy.

Ternary Phase Field Parameters

In Equation 4-10, ε (SI unit: 1/m) is a parameter controlling the interface thickness, M_0 (SI unit: m^3/s) is a molecular mobility parameter, and the parameter Σ_T is defined as

$$\frac{3}{\Sigma_T} = \frac{1}{\Sigma_A} + \frac{1}{\Sigma_B} + \frac{1}{\Sigma_C} \tag{4-15}$$

When using the interface it is recommended that the parameter ε is given a value in the same order as the elements in the regions passed by the fluid-fluid interfaces. The mobility determines the time scale of the Cahn–Hilliard diffusion and must be large enough to retain a constant interfacial thickness, but small enough to avoid damping the convective transport. In order to ensure that the mobility is in the correct range, it is recommended to apply a mobility parameter such that the following holds approximately

$$M_0 = L_c U_c \varepsilon \cdot 10^{-2} \tag{4-16}$$

where L_c and U_c are the characteristic length and velocity scales of the system at hand.

SURFACE TENSION

The surface tension force applied in the momentum equations (Equation 4-3) as a body force computed from the generalized chemical potentials:

$$\mathbf{F}_{\mathrm{st}} = \sum_{i = \mathrm{A}, B, C} \eta_i \nabla \phi_i \tag{4-17}$$

Reference for the Three-Phase Flow, Phase Field Interface

1. F. Boyer, C. Lapuerta, S. Minjeaud, B. Piar, and M. Quintard, "Cahn-Hilliard/Navier–Stokes model for the simulation of three-phase flows," *Transport in Porous Media*, vol. 28, pp. 463–484, 2010.

Theory for the Two-Phase Flow, Moving Mesh Interface

The Laminar Two-Phase Flow, Moving Mesh Interface can be used to model the flow of two different, immiscible fluids, when the exact position of the interface is of interest. The interface position is tracked by a moving mesh, with boundary conditions that account for surface tension and wetting, as well as mass transport across the interface.

In this section:

- Domain Level Fluid Flow
- About the Moving Mesh
- About the Fluid Interface Boundary Conditions
- Contact Angle Boundary Conditions
- References for the Two-Phase Flow, Moving Mesh Interface

Domain Level Fluid Flow

Two Phase Flow Moving Mesh interface is a predefined physics interface coupling between a Single-Phase Flow interface and the Moving Mesh interface. Within the domains corresponding to individual phases the fluid flow is solved using the Navier–Stokes equations as in the Laminar Flow interface. The general form for the isothermal Navier–Stokes equations is:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \cdot [-p\mathbf{I} + \tau] + \mathbf{F}$$

where:

- ρ is the density (SI unit: kg/m^3)
- $\mathbf{u}$ is the velocity vector (SI unit: m/s)
- p is pressure (SI unit: Pa)
- $\mathbf{F}$ is the volume force vector (SI unit: N/m^3)

- τ is the viscous stress tensor (SI unit: Pa).

For a Newtonian fluid the viscous stress tensor, τ, is given by:

$$\tau = 2\mu\mathbf{S} - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I} \tag{4-18}$$

The dynamic viscosity μ (SI unit: Pa·s) is allowed to depend on the thermodynamic state but not on the velocity field.

Theory for the Single-Phase Flow Interfaces

About the Moving Mesh

The mesh within the fluid flow domain is deformed to account for the movement of the interface between the two fluids. The software perturbs the mesh nodes so they conform with the moving interface and with other moving or stationary boundaries in the model. The boundary displacement is propagated throughout the domain to obtain a smooth mesh deformation everywhere. This is done by solving equations for the mesh displacements (a Laplace, Winslow, or hyperelastic smoothing equation). Taking two dimensions as an example, a location in the deformed mesh with coordinates (x, y) can be related to its coordinates in the original undeformed mesh (X, Y) by a function of the form:

$$x = x(X, Y, t), \qquad y = y(X, Y, t)$$

The original, undeformed, mesh is referred to as the *material frame* (or reference frame) whilst the deformed mesh is called the *spatial frame*. COMSOL Multiphysics also defines *geometry* and *mesh frames*, which are coincident with the material frame for this physics interface.

The fluid flow equations (along with other coupled equations such as electric fields or chemical species transport) are solved in the spatial frame in which the mesh is perturbed. The movement of the phase boundary is therefore accounted for in these interfaces.

Deformed Geometry and Moving Mesh in the *COMSOL Multiphysics Reference Manual*

About the Fluid Interface Boundary Conditions

The interfaces between phases are tracked with specific boundary conditions for the mesh displacement and the fluid flow. Two options are available — Free Surface and Fluid-Fluid Interface. The Free Surface boundary condition is appropriate when the viscosity of the external fluid is negligible compared to that of the internal fluid. In this case the pressure of the external fluid is the only parameter required to model the fluid and the flow is not solved for in the external fluid. For a fluid-fluid interface the flow is solved for both phases.

FLUID-FLUID INTERFACE

The boundary conditions applied at an interface between two immiscible fluids, fluid 1 and fluid 2 (see Figure 4-2), are given by (Ref. 1):

$$\mathbf{u}_1 = \mathbf{u}_2 + \left(\frac{1}{\rho_1} - \frac{1}{\rho_2}\right) M_f \mathbf{n}_i \tag{4-19}$$

$$\mathbf{n}_i \cdot \tau_2 = \mathbf{n}_i \cdot \tau_1 + \mathbf{f}_{st} \tag{4-20}$$

$$\mathbf{u}_{\text{mesh}} = \left(\mathbf{u}_1 \cdot \mathbf{n}_i - \frac{M_f}{\rho_1}\right) \mathbf{n}_i \tag{4-21}$$

where $\mathbf{u}_1$ and $\mathbf{u}_2$ are the velocities of the fluids 1 and 2 respectively, $\mathbf{u}_{\text{mesh}}$ is the velocity of the mesh at the interface between the two fluids, $\mathbf{n}_i$ is the normal of the interface (outward from the domain of fluid 1), τ_1 and τ_2 are the total stress tensors in domains 1 and 2 respectively, $\mathbf{f}_{st}$ is the force per unit area due to the surface tension and M_f is the mass flux across the interface (SI unit: kg/(m^{2}s)).

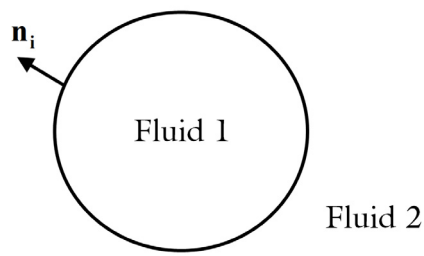


Figure 4-2: Definition of fluid 1 and fluid 2 and the interface normal.

The tangential components of Equation 4-19 enforce a no-slip condition between the fluids at the boundary. In the absence of mass transfer across the boundary, Equation 4-19 and Equation 4-21 ensure that the fluid velocity normal to the boundary is equal to the velocity of the interface. When mass transfer occurs these equations result from conservation of mass and are easily derived in the frame where the boundary is stationary.

The components of the total stress tensor, τ_{uv}, represent the uth component of the force per unit area perpendicular to the v direction. $\mathbf{n}\cdot\tau = \mathbf{n}_v\tau_{uv}$ (using the summation convention) is therefore interpreted as the force per unit area acting on the boundary - in general this is not normal to the boundary. Equation 4-20 therefore expresses the force balance on the interface between the two fluids.

	Two boundary conditions (Equation 4-19 and Equation 4-20) are necessary to couple the two domains as there are two separate sets of Navier–Stokes equations, one set for each of the domains.

The force due to the surface tension is given by the following expression:

$$\mathbf{f}_{st} = \sigma(\nabla_s \cdot \mathbf{n}_i)\mathbf{n}_i - \nabla_s\sigma \tag{4-22}$$

where ∇_s is the surface gradient operator ($\nabla_s = (\mathbf{I} - \mathbf{n}_i\,\mathbf{n}_i^T)\nabla$, where $\mathbf{I}$ is the identity matrix) and σ is the surface tension at the interface.

In the two dimensional case it is straightforward to see the physical origin of Equation 4-22. Consider an element of the surface of unit depth into the page as shown in Figure 4-3. The normal force per unit area $\mathbf{F}_n$ on the element in the limit $\delta s \to 0$ is:

$$\mathbf{F}_n\delta s = (\sigma + \delta\sigma)\sin(\delta\theta) \to \sigma\delta\theta$$

Because $R\delta\theta \to \delta s$ in the limit,

$$\mathbf{F}_n = \frac{\sigma}{R}$$

The quantity $\nabla_s\cdot\mathbf{n}_i$ in the first term on the right-hand side of Equation 4-22 is related to the mean curvature, κ, of the surface by the equation $\kappa = -\nabla_s\cdot\mathbf{n}_i$. In two dimensions the mean curvature $\kappa = -1/R$ so $\nabla_s\cdot\mathbf{n}_i = 1/R$. The first term in Equation 4-22 is therefore the normal force per unit area acting on the boundary due to the surface tension.

The tangential force per unit area, $\mathbf{F}_t$, acting on the interface in Figure 4-3 can be obtained from the force balance along the direction of δs in the limit $\delta s \to 0$:

$$\mathbf{F}_t \delta s = (\sigma + \delta\sigma)\cos(\delta\theta) - \sigma \to (\sigma + \delta\sigma) - \sigma$$

$$\mathbf{F}_t \to \frac{(\sigma + \delta\sigma) - \sigma}{\delta s}$$

This is equivalent to the second term on the right of Equation 4-22.

To obtain additional insight into the boundary condition, it is helpful to rewrite Equation 4-20 as

$$\mathbf{n}_i \cdot ((p_1 - p_2)I - \mu_1(\nabla\mathbf{u}_1 - (\nabla\mathbf{u}_1)^T) + \mu_2(\nabla\mathbf{u}_2 - (\nabla\mathbf{u}_2)^T)) = \sigma(\nabla_s \cdot \mathbf{n}_i)\mathbf{n}_i - \nabla_s\sigma$$

assuming Newtonian fluids with viscosities μ_1 and μ_2 for fluids 1 and 2, respectively, and that p_1 and p_2 are the pressures in the respective fluids adjacent to the boundary. This equation expresses the equality of two vector quantities. It is instructive to consider the components perpendicular and tangential to the boundary. In the direction of the boundary normal

$$p_1 - p_2 + \mathbf{n}_i \cdot (\mu_2(\nabla\mathbf{u}_2 - (\nabla\mathbf{u}_2)^T) - \mu_1(\nabla\mathbf{u}_1 - (\nabla\mathbf{u}_1)^T)) \cdot \mathbf{n}_i = \sigma(\nabla_s \cdot \mathbf{n}_i)\mathbf{n}_i \quad (4\text{-}23)$$

whereas in the tangential direction, $\mathbf{t}_i$,

$$\mathbf{n}_i \cdot (\mu_2(\nabla\mathbf{u}_2 - (\nabla\mathbf{u}_2)^T) - \mu_1(\nabla\mathbf{u}_1 - (\nabla\mathbf{u}_1)^T)) \cdot \mathbf{t}_i = |\nabla_s\sigma| \quad (4\text{-}24)$$

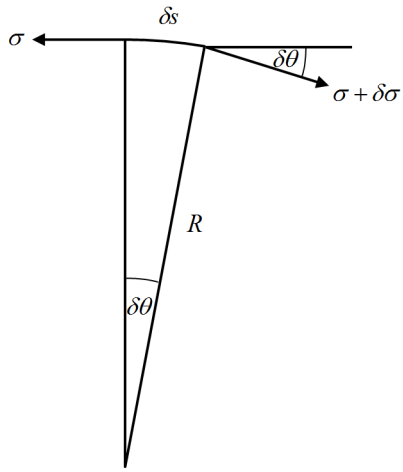


Figure 4-3: Diagrammatic representation of the forces acting on an element of a two-dimensional curved surface.

For the case of a static interface, Equation 4-23 expresses the pressure difference across the interface that results from its curvature. For a moving interface, the surface tension balances the difference in the total normal stress on either side of the interface.

Equation 4-24 involves only velocity gradients and the gradient of the surface tension. The implication of this is that surface tension gradients always drive motion; this is known as the *Marangoni effect*.

FREE SURFACE

It is often the case that the viscosity of fluid 1 is significantly greater than that of fluid 2 (for example for a liquid-vapor interface). In this case, the viscosity terms in the total stress from fluid 2 can be neglected and Equation 4-20 becomes:

$$\mathbf{n}_i \cdot \tau_1 = -p_{\text{ext}}\mathbf{n}_i + \mathbf{f}_{st} \tag{4-25}$$

The outer fluid (fluid 2) now enters the equation system only through the pressure term and the system can be represented by a domain consisting solely of the fluid 1 domain with an expression (or constant value) for the external pressure, p_{ext}, in the fluid 2 domain. Since the velocity in fluid 2 does not affect fluid 1, fluid 2 does not need to be explicitly modeled and Equation 4-19 can be dropped.

Contact Angle Boundary Conditions

At a three-phase boundary, it is necessary to add force terms on the boundary to ensure that the fluid maintains a consistent contact angle. Additionally the Wall boundary condition with the Navier Slip option must be used on the walls. The forces acting on the contact point are applied to the model by the Contact Angle node.

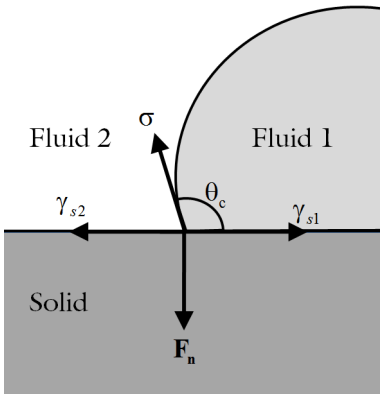


Figure 4-4: Forces per unit length acting on a fluid-fluid interface at a three phase boundary with a solid wall. The surface tension force per unit length, σ, is balanced by a reaction force per unit length at the surface, $\mathbf{F}_n$*, and by the forces generated by the surface energies of the two phases at the interface:* γ_{s1} *and* γ_{s2}*.*

In equilibrium, the surface tension forces and the normal restoring force from the surface are in balance at a constant contact angle (θ_c), as shown in Figure 4-4. This equilibrium is expressed by Young's equation, which considers the components of the forces in the plane of the surface:

$$\sigma\cos(\theta_c) + \gamma_{s1} = \gamma_{s2} \tag{4-26}$$

where σ is the surface tension force between the two fluids, γ_{s1} is the surface energy density on the fluid 1 — solid interface and γ_{s2} is the surface energy density on the fluid 2 — solid interface.

There is still debate in the literature as to precisely what occurs in nonequilibrium situations (for example, drop impact) when the physical contact angle deviates from the contact angle specified by a simple application of Young's equation. A simple approach is to assume that the unbalanced part of the in plane Young Force acts on the fluid to move the contact angle toward its equilibrium value (Ref. 2). COMSOL

Multiphysics employs this approach as it is physically motivated and is consistent with the allowed form of the boundary condition from thermodynamics (Ref. 3 and Ref. 4).

The normal force balance at the solid surface is handled by the wall boundary condition, which automatically prevents fluid flow across the solid boundary by the application of a constraint force. The contact angle feature applies a force on the fluid at the interface, $\mathbf{f}_{wf}$, with magnitude:

$$\mathbf{f}_{wf} = \sigma(\cos(\theta_c) - \cos(\theta))\mathbf{m}_s$$

where θ is the actual contact angle and $\mathbf{m}_s$ is the binormal to the solid surface, as defined in Figure 4-5.

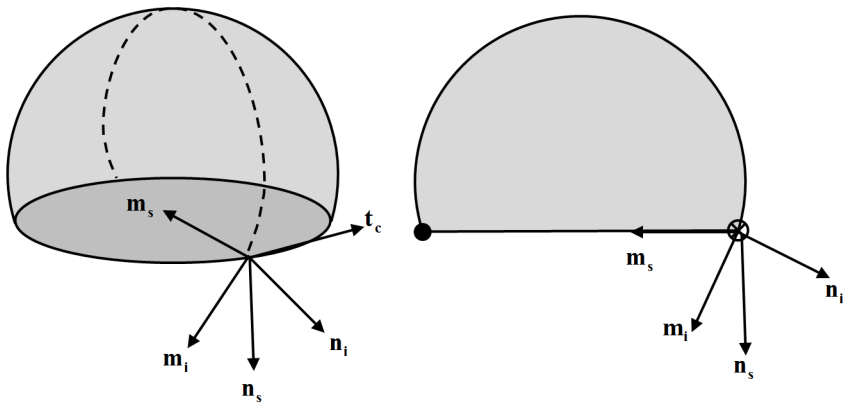


Figure 4-5: Diagram showing normal and tangential vectors defined on the interface between two fluids and a solid surface in 3D (left) and 2D (right). The following vectors are defined: $\mathbf{n}_i$*, the fluid-fluid interface unit normal;* $\mathbf{n}_s$*, the solid surface unit normal;* $\mathbf{t}_c$*, the tangent to the three-phase contact line; and* $\mathbf{m}_i$ *and* $\mathbf{m}_s$*, the two unit binormals, which are defined as* $\mathbf{m}_i = \mathbf{t}_c \times \mathbf{n}_i$ *and* $\mathbf{m}_s = \mathbf{t}_c \times \mathbf{n}_s$*, respectively.*

References for the Two-Phase Flow, Moving Mesh Interface

1. R. Scardovelli and S. Zaleski, "Direct Numerical Simulation of Free Surface and Interfacial Flow," *Annu. Rev. Fluid Mech.*, vol. 31, pp. 567–603, 1999.

2. J. Gerbeau and T. Lelièvre, "Generalized Navier Boundary Condition and Geometric Conservation Law for Surface Tension," *Comput. Methods Appl. Mech. Eng.*, vol. 198, pp. 644–656, 2009.

3. W. Ren and E. Weinan, "Boundary Conditions for the Moving Contact Line Problem", *Phys. Fluids*, vol. 19, p. 022101, 2007.

4. W. Ren and D. Hu, "Continuum Models for the Contact Line Problem", *Phys. Fluids*, vol. 22, p. 102103, 2010.

5. J. J. Jasper, "The Surface Tension of Pure Liquid Compounds", *J. Phys. Chem. Ref. Data.*, vol. 1, no. 4, pp. 841-1009, 1972.

6. R. C. Weast, ed.,"CRC Handbook of Chemistry and Physics", ed. 69, MIT Press, 1988.

7. A. G. Gaonkar, "Interfacial Tensions of Vegetable Oil/Water Systems: Effect of Oil Purification", *J. Am. Oil Chem. Soc.*, vol. 66, no. 8, pp. 1090-1092, 1989.

5

Mathematics, Moving Interfaces

The Level Set and Phase Field in Fluids Moving Interfaces are available under the **Mathematics** > **Moving Interface** branch ( ) when adding interfaces. See Modeling Microfluidic Fluid Flows to help you select which interface to use.

- The Level Set Interface
- The Phase Field in Fluids Interface
- The Ternary Phase Field Interface
- Theory for the Level Set Interface
- Theory for the Phase Field in Fluids Interface
- Theory for the Ternary Phase Field Interface

The Level Set Interface

In this section:

- The Level Set Interface
- The Level Set in Porous Media Interface
- Domain, Boundary, and Pair Nodes for the Level Set Interface

The Level Set Interface

The **Level Set (ls)** interface ( ), found under the **Mathematics** > **Moving Interface** branch ( ) when adding an interface, is used to track moving interfaces in fluid-flow models by solving a transport equation for the level set function. Simulations using the **Level Set** interface are always time dependent because the position of an interface almost always depends on its history.

The main node is the Level Set Model feature, which adds the level set equation and provides an interface for defining the level set properties and the velocity field.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Level Set Model**, **No Flow** (the default boundary condition), **Initial Values**, and **Initial Values, Fluid 2**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions. You can also right-click **Level Set** to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `ls`.

STABILIZATION

To display this sections, click the **Show More Options** button ( ) and select **Stabilization** in the **Show More Options** dialog.

There are two stabilization methods available — **Streamline diffusion** and **Crosswind diffusion**. Both are active by default and should remain selected for optimal performance.

ADVANCED SETTINGS

To display this sections, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog.

Specify the **Convective term** as **Nonconservative form** (default) or **Conservative form**.

DISCRETIZATION

By default, the Level Set interface uses **Linear** elements. When coupling the physics interface to a fluid flow interface by means of The Two-Phase Flow, Level Set Coupling Feature, exact conservation of the integral of ϕ is obtained using the nonconservative form provided that the discretization order of the level set variable is equal to or lower than the order of the pressure.

DEPENDENT VARIABLES

The dependent variable (field variable) is the **Level set variable** phi. The name can be changed but the names of fields and dependent variables must be unique within a model.

- Conservative and Nonconservative Form
- Domain, Boundary, and Pair Nodes for the Level Set Interface
- Theory for the Level Set Interface
- Theory for the Level Set and Phase Field Interfaces

The Level Set in Porous Media Interface

The **Level Set in Porous Media (ls)** interface ( ), found under the **Mathematics** > **Moving Interface** branch ( ) when adding an interface, is used to track moving interfaces in fluid-flow through porous media models by solving a transport equation for the level set function. Simulations using the **Level Set in Porous Media** interface are always time dependent since the position of an interface almost always depends on its history.

The main node is the Porous Medium Level Set Model feature, which adds the level set equation and provides interfaces for defining the level set properties, the velocity field and the porosity of the porous matrix.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Porous Medium**, **No Flow** (the default boundary condition), **Initial Values**, and **Initial Values, Fluid 2**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions. You can also right-click **Level Set in Porous Media** to select physics features from the context menu.

SETTINGS

The rest of the settings are the same as for the **Level Set** interface.

Domain, Boundary, and Pair Nodes for the Level Set Interface

The Level Set Interface has the following domain, boundary, and pair nodes described.

- Continuity
- Initial Values
- Inlet
- Level Set Model
- No Flow
- Open Boundary
- Outlet[1]
- Periodic Condition (see Periodic Boundary Conditions in the *COMSOL Multiphysics Reference Manual*)
- Porous Matrix
- Porous Medium
- Symmetry[1]
- Thin Barrier

[1] Described for the Laminar Flow interface.

	Boundary conditions for axial symmetry boundaries are not required. For the symmetry axis at $r = 0$, the software automatically provides a suitable boundary condition and adds an **Axial Symmetry** node that is valid on the axial symmetry boundaries only.

!	In the *COMSOL Multiphysics Reference Manual* see Table 2-4 for links to common sections and Table 2-5 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Level Set Model

If the **Level Set Model** node is a domain feature under The Level Set Interface, it adds the following transport equation governing a level set function ϕ:

$$\frac{\partial\phi}{\partial t} + \mathbf{u}\cdot\nabla\phi = \gamma\nabla\cdot\left(\varepsilon_{ls}\nabla\phi - \phi(1-\phi)\frac{\nabla\phi}{|\nabla\phi|}\right)$$

If it is a domain subfeature under the Porous Medium domain feature, it adds the following equation:

$$\varepsilon_p\frac{\partial\phi}{\partial t} + \mathbf{u}\cdot\nabla\phi = \gamma\nabla\cdot\left(\varepsilon_{ls}\nabla\phi - \phi(1-\phi)\frac{\nabla\phi}{|\nabla\phi|}\right)$$

In both cases, the **Level Set Model** node provides the options to define the associated level set parameters and the velocity field.

LEVEL SET PARAMETERS

Enter a value or expression for the **Reinitialization parameter** γ (SI unit: m/s). The default is 1 m/s.

Enter a value or expression for the **Parameter controlling interface thickness** ε_{ls} (SI unit: m). The default expression is `ls.ep_default`, a value proportional to the maximum element size with a proportionality factor dependent on the ratio of the maximum and minimum element sizes in the domain.

CONVECTION

Enter values or expressions for the components (u, v, and w in 3D, for example) of the **Velocity field** $\mathbf{u}$ (SI unit: m/s). The applied velocity field transports the level set function through convection.

Porous Medium

The **Porous Medium** node adds the level set equation. It has two default subfeatures — the Level Set Model feature where the reinitialization parameter γ (SI unit: m/s) and the parameter controlling the interface thickness ε_{ls} (SI unit: m) are defined, and the Porous Matrix feature where the porosity ε_p (dimensionless) is specified.

Porous Matrix

This node contains inputs for the material properties of the solid matrix of the Porous Medium parent node.

MATRIX PROPERTIES

The **Porosity** ε_p (a dimensionless number between 0 and 1) uses by default the value **From material**. For **User defined** the default is 1.

Initial Values

Use the **Initial Values** node to define the initial values of the level set variable.

INITIAL VALUES

The initial positions of the two fluids, and consequently the separating interface, can be specified in two ways. The level set function can be specified explicitly using any type of variable or expression. Alternatively, the fluid occupying the current domain selection can be specified. Using the former method, a Time Dependent study step can directly be solved. Using the latter method, a Phase Initialization study step is needed in order to initialize the level set function across the fluid-fluid interface.

Specify the **Level set variable** as one of the following:

- To specify the fluid occupying the domain, select **Specify phase** (default). Then select the checkbox **Fluid 1 ($\phi = 0$)** or **Fluid 2 ($\phi = 1$)**.
- For **User defined** enter a value or expression for the level set variable ϕ.

!	If the **Phase Initialization** ( ) study step is being used, for the initialization to work it is crucial that there are two **Initial Values** nodes. One of the Initial Values nodes should use **Specify phase: Fluid 1 ($\phi = 0$)** and the other **Specify phase: Fluid 2 ($\phi = 1$)**. The initial fluid-fluid interface is then automatically placed on all interior boundaries between both phases. The smooth initialization is not used in domains with **User defined** initial values. See Initializing the Level Set Function.

Inlet

LEVEL SET CONDITION

Specify **Level Set Condition** according to one of the following options:

- **Fluid 1 ($\phi = 0$)**
- **Fluid 2 ($\phi = 1$)**
- **Specify level set function explicitly**

When the **Specify level set function explicitly** is selected, the level set function ϕ must be specified explicitly. The value must be in the range from 0 to 1, where the default is 0.

No Flow

The **No Flow** node adds a boundary condition that represents boundaries where there is no flow across the boundary. This is the default boundary condition.

Open Boundary

Use this node to set up transport across boundaries where both convective inflow and outflow can occur. On the parts of the boundary where fluid flows into the domain, an exterior value of the level set function is prescribed. On the remaining parts, where fluid flows out of the domain, a condition equivalent to the **Outflow** node is instead prescribed.

The direction of the flow across the boundary is typically calculated by a fluid flow interface and is provided as a model input to the Level Set interface.

LEVEL SET CONDITION

Specify **Level Set Condition** according to one of the following options:

- **Fluid 1 ($\phi = 0$)**
- **Fluid 2 ($\phi = 1$)**
- **Specify level set function explicitly**

When the **Specify level set function explicitly** is selected, the level set function ϕ must be specified explicitly. The value must be in the range from 0 to 1, where the default is 0.

Thin Barrier

The **Thin Barrier** feature is available on interior boundaries and introduces a discontinuity in the level set variable across the boundary. A No Flow condition is prescribed on each side. This node can be used to avoid meshing thin structures.

Continuity

The **Continuity** condition is suitable for pairs where the boundaries match; it prescribes that the level set variable is continuous across the pair.

The parts of the boundary where a source boundary lacks a corresponding destination boundary and vice versa will get conditions from other boundary conditions under the physics interface acting as fallback boundary conditions on the nonoverlapping parts. By default, the No Flow node is used as fallback unless another feature has been selected for the boundary.

About Pairs

LOCATION IN USER INTERFACE

Right-click the physics interface and select **Pairs** > **Continuity**.

Ribbon

Physics tab with the physics interface selected:

Pairs > **Continuity**

The Phase Field in Fluids Interface

The **Phase Field in Fluids (pf)** interface ( ), found under the **Mathematics** > **Moving Interface** branch ( ) when adding a physics interface, is used to track moving fluid-fluid interfaces by solving two transport equations, one for the phase field variable, ϕ, and one for the mixing energy density, ψ. The position of the interface is determined by minimizing the free energy.

The main node is the Phase Field Model feature, which adds the phase field equations and provides an interface for defining the phase field model properties.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Phase Field Model**, **Wetted Wall** (the default boundary condition), **Initial Values**, and **Initial Values, Fluid 2**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions. You can also right-click **Phase Field in Fluids** to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `pf`.

ADVANCED SETTINGS

To display this sections, click the **Show More Options** button ( ) and select **Advanced settings options** in the **Show More Options** dialog.

Specify the **Convective term** as **Nonconservative form** (default) or **Conservative form**.

DISCRETIZATION

By default, the Phase Field in Fluids interface uses **Linear** elements.

DEPENDENT VARIABLES

This interface defines the dependent variables (fields) **Phase field variable** ϕ and **Phase field help variable** ψ. If required, edit the name, but dependent variables must be unique within a model.

- Conservative and Nonconservative Forms
- Domain, Boundary, and Pair Nodes for the Phase Field in Fluids Interface
- Theory for the Phase Field in Fluids Interface

Domain, Boundary, and Pair Nodes for the Phase Field in Fluids Interface

The Phase Field in Fluids Interface includes the following domain, boundary, and pair nodes, listed in alphabetical order, available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

- Continuity
- Initial Values
- Inlet
- Interior Wetted Wall
- Outlet
- Periodic Condition (see Periodic Boundary Conditions in the *COMSOL Multiphysics Reference Manual*)
- Phase Field Model
- Symmetry
- Wetted Wall

In the *COMSOL Multiphysics Reference Manual* see Table 2-4 for links to common sections and Table 2-5 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Phase Field Model

The **Phase Field Model** node adds the equations described in The Equations for the Phase Field Method. The node defines the associated phase field parameters including surface tension and interface thickness.

PHASE FIELD PARAMETERS

Define the following phase field parameters. Enter a value or expression for the:

- **Surface tension coefficient** σ (SI unit: N/m).
- **Parameter controlling interface thickness** ε_{pf} (SI unit: m). The default expression is `pf.ep_default`, a value proportional to the maximum element size with a proportionality factor dependent on the ratio of the maximum and minimum element sizes in the domain.
- **Mobility tuning parameter** χ (SI unit: m·s/kg). This parameter determines the time scale of the Cahn–Hilliard diffusion and it thereby also governs the diffusion-related time scale for the interface. Select **User defined** (default) or **Calculate from velocity**. For **User defined** enter a value or expression for the mobility tuning parameter χ. The default is 1 m·s/kg, which is a good starting point for most models.

  For **Calculate from velocity** enter a value for the expected velocity at the interface U (SI unit: m/s). χ is then computed as:

$$\chi = \frac{Uh_{\max}}{3\sqrt{2}\sigma\varepsilon}$$

  where $h_{\max}$ is the largest mesh cell size.

	Keep the χ parameter value large enough to maintain a constant interface thickness but still low enough to not damp the convective motion. A too high mobility can also lead to excessive diffusion of droplets.

EXTERNAL FREE ENERGY

Add a source of external free energy to the phase field equations. This modifies the last term on the right-hand side of the equation:

$$\psi = -\nabla \cdot \varepsilon^2 \nabla\phi + (\phi^2 - 1)\phi + \left(\frac{\varepsilon^2}{\lambda}\right)\frac{\partial f}{\partial \phi}$$

The external free energy f (SI unit: J/m^3) is a user-defined free energy. In most cases, the external free energy can be set to zero. Manually differentiate the expression for the external free energy with respect to ϕ and then enter it into the **ϕ-derivative of external free energy** field $\partial f/\partial\phi$.

CONVECTION

Enter values or expressions for the components (u, v, and w in 3D, for example) of the **Velocity field** u (SI unit: m/s). The applied velocity field transports the phase field variables through convection.

	Additional Sources of Free Energy

Initial Values

Use the **Initial Values** node to define the initial values of the phase field variable.

INITIAL VALUES

The initial positions of the two fluids, and consequently the fluid-fluid interface, can be specified in two ways. The phase field variable can be specified explicitly, using any type of variable or expression. Alternatively the fluid occupying the current domain selection can be specified. Using the former method, a Time Dependent study step can directly be solved. Using the latter method, a Phase Initialization study step is needed in order to initialize the phase field function across the fluid-fluid interface.

Specify the **Phase field variable** as one of the following:

- To specify the fluid occupying the domain, select **Specify phase** (default). Then select the checkbox **Fluid 1** ($\phi = -1$) or **Fluid 2** ($\phi = 1$).
- For **User defined** enter a value or expression for the phase field variable ϕ.

!	If the **Phase Initialization** ( ) study step is being used, for the initialization to work it is crucial that there are two **Initial Values** nodes. One of the Initial Values nodes is set to **Specify phase: Fluid 1 ($\phi = -1$)** and the other to **Specify phase: Fluid 2 ($\phi = 1$)**. The initial fluid-fluid interface is then automatically placed on all interior boundaries between both phases. The smooth initialization is not used in domains with **User defined** initial values.

Inlet

SETTINGS

Specify **Phase field Condition** according to one of the following options:

- **Fluid 1 ($\phi = -1$)**
- **Fluid 2 ($\phi = 1$)**
- **Specify phase field function explicitly**

When **Specify phase field function explicitly** is selected, the phase field function ϕ must be specified in the entire domain. The value must be in the range from –1 to 1, where the default is 1.

Wetted Wall

The **Wetted Wall** node is the default boundary condition representing wetted walls. Along a wetted wall the contact angle for the fluid, θ_w, is specified, and across it, the mass flow is zero. This is prescribed by

$$\mathbf{n} \cdot \varepsilon^2 \nabla\phi = \varepsilon^2 \cos(\theta_w)|\nabla\phi|$$

in combination with

$$\mathbf{n} \cdot \frac{\gamma\lambda}{\varepsilon^2}\nabla\psi = 0$$

The contact angle θ_w can be defined directly or from Young's equation, which considers the components of the forces in the plane of the surface:

$$\sigma\cos(\theta_w) + \gamma_{s2} = \gamma_{s1} \tag{5-1}$$

where γ_{s1} is the surface energy density on the fluid 1 — solid (wall) interface and γ_{s2} is the surface energy density on the fluid 2 — solid (wall) interface.

WETTED WALL

Select an option from the **Specify contact angle list** — **Directly** (the default) or **Through Young's equation**. For **Directly** enter a value or expression for the **Contact angle** θ_w (SI unit: rad). The default value is $\pi/2$ radians. For **Through Young's equation** enter values or expressions for **Phase 1-Solid surface energy density** γ_{s1} (SI unit: J/m^2) and **Phase 2-Solid surface energy density** γ_{s2} (SI unit: J/m^2).

Interior Wetted Wall

The **Interior Wetted Wall** feature is available on interior boundaries. It is similar to the Wetted Wall condition except that it applies on both sides of an interior boundary and introduces a discontinuity of the phase field variables across the boundary. This node can be used to avoid meshing thin structures.

Along an interior wetted wall the contact angle for the fluid, θ_w, is specified on both sides of the boundary, and across it, the mass flow is zero.

WETTED WALL

Enter a value or expression for the **Contact angle** θ_w. The default value is $\pi/2$ rad.

Continuity

The **Continuity** condition is suitable for pairs where the boundaries match; it prescribes that the phase field variables are continuous across the pair.

The parts of the boundary where a source boundary lacks a corresponding destination boundary and vice versa will get conditions from other boundary conditions under the physics interface acting as fallback boundary conditions on the nonoverlapping parts. By default, the Wetted Wall node is used as fallback unless another feature has been selected for the boundary.

About Pairs

LOCATION IN USER INTERFACE

Right-click the physics interface and select **Pairs** > **Continuity**.

Ribbon

Physics tab with the physics interface selected:

Pairs > **Continuity**

The Ternary Phase Field Interface

The **Ternary Phase Field (terpf)** interface ( ), found under the **Mathematics** > **Moving Interface** branch ( ) when adding a physics interface, is used to track moving interfaces separating three different phases. The interface solves four transport equations: two equations governing phase field variables, ϕ_A and ϕ_B, and two equations for the corresponding generalized chemical potentials, η_A and η_B. The position of the interfaces are determined by minimization of the free energy.

The phase field variables are defined such that they represent the volume fraction of the respective phase. The volume fraction of the third phase not solved for, but computed from the natural constraint that the sum of the volume fractions of all phases is one.

The main node of the interface is the Phase Field Model feature, which adds the phase field equations and provides an interface for defining the phase field model properties such as surface tensions and parameters controlling the interface thickness.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Mixture Properties**, **Wetted Wall** and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions. You can also right-click **Ternary Phase Field** to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `terpf`.

DEPENDENT VARIABLES

This interface defines the dependent variables (fields):

- **Phase field variable, fluid A** `phiA`
- **Phase field variable, fluid B** `phiB`

- **Generalized chemical potential of fluid A** `etaA`
- **Generalized chemical potential of fluid B** `etaB`

If required, edit the any of the names, but dependent variables must be unique within a model.

	Theory for the Ternary Phase Field Interface

Domain, Boundary, and Pair Nodes for the Ternary Phase Field Interface

The Ternary Phase Field Interface includes the following domain, boundary, and pair nodes, listed in alphabetical order, available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or by right-clicking the interface node to access the context menu (all users).

- Initial Values
- Inlet
- Outlet
- Phase Field Model
- Symmetry
- Wetted Wall

Mixture Properties

The **Mixture Properties** node adds the equations described in The Equations of the Ternary Phase Field Method. The node defines the associated phase field parameters, including the surface tension coefficients and parameters controlling the thickness of the interfaces.

MODEL INPUTS

The surface tension coefficients can be defined through user inputs, variables, or by selecting a material. For the latter option, an additional input, the temperature, may be required to define these properties.

Temperature

By default, the **Temperature** model input is set to **Common model input**, and the temperature is controlled from Default Model Inputs under **Global Definitions** or by a locally defined Model Input. If a Heat Transfer interface is included in the component,

it controls the temperature **Common model input**. Alternatively, the temperature field can be selected from another physics interface. All physics interfaces have their own tags (**Name**). For example, if a Heat Transfer in Fluids interface is included in the component, the **Temperature (ht)** option is available for T.

You can also select **User defined** from the **Temperature** model input in order to manually prescribe T

	Model Inputs and Multiphysics Couplings in the *COMSOL Multiphysics Reference Manual*

PHASE FIELD PARAMETERS

Define the following phase field parameters. Enter a value or expression for the:

Parameter controlling interface thickness ε. The default expression is `terpf.ep_default*sqrt(2)`, a value proportional to the maximum element size with a proportionality factor dependent on the ratio of the maximum and minimum element sizes in the domain.

- **Mobility tuning parameter** M_0. This parameter determines the time scale of the Cahn–Hilliard diffusion and it thereby also governs the diffusion-related time scale for the interface. Keep the mobility tuning parameter value large enough to maintain a constant interface thickness but still low enough to not damp the convective motion. A too high mobility can also lead to excessive diffusion of droplets. By default, M_0 is set to $1\cdot10^{-4}$ m^3/s, which is a good starting point for most models.
- **Additional free bulk energy** Λ. When needed, add a user-defined expression for the additional bulk energy.

SURFACE TENSION

Specify the surface tension coefficients for the three types of interfaces present.

- To use a predefined expression, select **Library coefficient, liquid/gas interface** or **Library coefficient, liquid/liquid interface.** Then select an option from the list that displays below (**Water/Air**, **Glycerol/Air**, and so forth).
- For **User defined**, enter a value or expression for the surface tension coefficient.

The predefined correlations are based on the data in Ref. 3, Ref. 4, and Ref. 5.

CONVECTION

Enter values or expressions for the components (u, v, and w in 3D, for example) of the **Velocity field** u. The applied velocity field transports the phase field variables through convection.

Initial Values

The **Initial Values** node adds initial values for the phase field variables that can serve as initial conditions for a transient simulation.

INITIAL VALUES

Enter initial values or expressions for **Phase field variable A** and the **Phase field variable B** corresponding to the mass fraction of the respective phase. The value must be in the range from 0 to 1.

Inlet

This condition should be used on boundaries for which there is a net convective flow of the phases into the adjacent domain.

INLET

Specify phase field variables, corresponding to the volume fractions, of phase A and phase B. The value must be in the range from 0 to 1. The volume fraction of phase C will be evaluated such that the sum of all mass fractions equals one.

Mathematically this boundary condition imposes

$$\phi_i = \phi_{i,0}, \ \mathbf{n} \cdot \frac{M_0}{\Sigma_i} \nabla \eta_i = 0$$

for phases $i = A$ and B.

Outlet

This condition should be used on boundaries for which there is a net convective outflow from the domain.

Mathematically this boundary condition imposes

$$\mathbf{n} \cdot \frac{M_0}{\Sigma_i} \nabla \eta_i = 0$$

for phases $i = A$ and B.

Symmetry

Use this condition on boundaries that represent a geometrical symmetry line across which the flow of the fluid phases is zero.

Mathematically this boundary condition imposes

$$\mathbf{n} \cdot \frac{M_0}{\Sigma_i} \nabla \eta_i = 0$$

for phases $i = A$ and B.

Wetted Wall

Use this node to represent a solid wall along which the contact angles between the separating interfaces and the wall should be prescribed.

WETTED WALL

Enter values or expressions for the contact angles for the three interfaces types:

- The **Contact angle of interface from phase A to phase C** θ_α.
- The **Contact angle of interface from phase B to phase C** θ_β.
- The **Contact angle of interface from phase A to phase B** θ_γ.

The definition of the contact angles with respect to the wall are shown in the figure below.

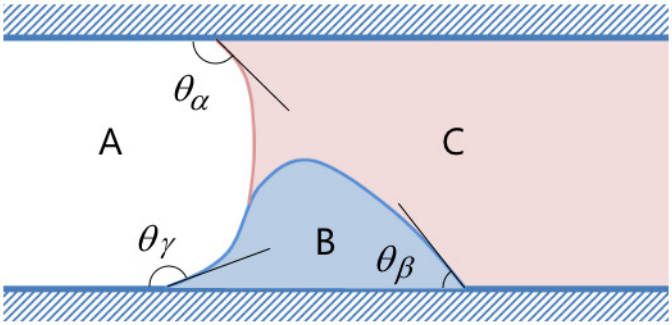


Figure 5-1: Definitions of the contact angels in the Wetted Wall feature of the Ternary Phase Field interface.

Theory for the Level Set Interface

Fluid flow with moving interfaces or boundaries occur in a number of different applications, such as *fluid-structure interaction*, multiphase flows, and flexible membranes moving in a liquid. One way to track moving interfaces is to use a level set method. A certain contour line of the globally defined function, the level set function, then represents the interface between the phases. For The Level Set Interface the fluid-fluid interface can be advected with an arbitrary velocity field.

In this section:

- The Level Set Method
- Conservative and Nonconservative Form
- Initializing the Level Set Function
- Variables For Geometric Properties of the Interface
- Reference for the Level Set Interface

The Level Set Method

The *level set method* is a technique to represent moving interfaces or boundaries using a fixed mesh. It is useful for problems where the computational domain can be divided into two domains separated by an interface. Each of the two domains can consist of several parts. Figure 5-2 shows an example where one of the domains consists of two separated parts. The interface is represented by a certain level set or isocontour of a globally defined function, the level set function ϕ. In COMSOL Multiphysics, ϕ is a smooth step function that equals zero (0) in one domain and one (1) in the other. Across the interface, there is a smooth transition from zero to one. The interface is

defined by the 0.5 isocontour, or level set, of ϕ. Figure 5-3 shows the level set representation of the interface in Figure 5-2.

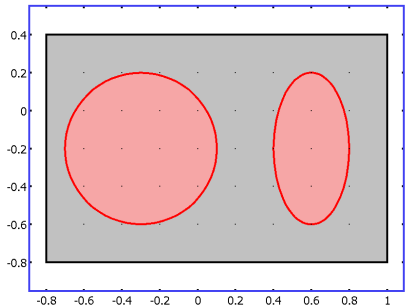


Figure 5-2: An example of two domains divided by an interface. In this case, one of the domains consists of two parts. Figure 5-3 *shows the corresponding level set representation.*

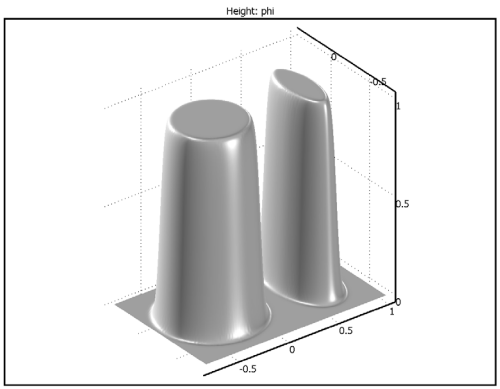


Figure 5-3: A surface plot of the level set function corresponding to Figure 5-2.

The physics interface solves Equation 5-2 in order to move the interface with the velocity field $\mathbf{u}$:

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \gamma \nabla \cdot \left(\varepsilon_{ls} \nabla \phi - \phi(1-\phi) \frac{\nabla \phi}{|\nabla \phi|} \right) \tag{5-2}$$

The terms on the left-hand side give the correct motion of the interface, while those on the right-hand side are necessary for numerical stability. The parameter, ε_{ls}, determines the thickness of the region where ϕ varies smoothly from zero to one and is typically of the same order as the size of the elements of the mesh. By default, ε_{ls} is

constant within each domain and proportional to the largest value of the mesh size, h, within the domain. The parameter γ determines the amount of reinitialization or stabilization of the level set function. It needs to be tuned for each specific problem. If γ is too small, the thickness of the interface might not remain constant and oscillations in ϕ can appear because of numerical instabilities. On the other hand, if γ is too large the interface moves incorrectly. A suitable value for γ is the maximum magnitude of the velocity field $\mathbf{u}$.

Conservative and Nonconservative Form

If the velocity is divergence free, that is, if

$$\nabla \cdot \mathbf{u} = 0 \tag{5-3}$$

the volume (area for 2D problems) bounded by the interface should be conserved if there is no inflow or outflow through the boundaries. To obtain exact numerical conservation in cases where Equation 5-3 is not fully satisfied, switch to the conservative form

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\mathbf{u}\phi) = \gamma \nabla \cdot \left(\varepsilon_{ls} \nabla \phi - \phi(1-\phi) \frac{\nabla \phi}{|\nabla \phi|} \right) \tag{5-4}$$

in Settings window for The Level Set Interface.

Using the conservative level set form, exact numerical conservation of the integral of ϕ is obtained. However, the nonconservative form is better suited for numerical calculations and usually converges more easily. The nonconservative form, which is the default form, only conserves the integral of the level set function approximately, but this level of conservation is sufficient for most applications.

When the Level Set interface is coupled to a fluid-flow interface by means of The Two-Phase Flow, Level Set Coupling Feature, exact conservation of the integral of ϕ is obtained using the nonconservative form, provided that the discretization order of the level set variable is equal to or lower than the order of the pressure.

Rising Bubble: Application Library path
Microfluidics_Module/Two-Phase_Flow/rising_bubble_2daxi

The Level Set Equation in Porous Domains

In a porous domain, the equation that determines the evolution of the interface is

$$\frac{\partial\phi}{\partial t} + \mathbf{u}_{\text{pore}} \cdot \nabla\phi = \gamma\nabla \cdot \left(\varepsilon_{\text{ls}}\nabla\phi - \phi(1-\phi)\frac{\nabla\phi}{|\nabla\phi|}\right) \tag{5-5}$$

Here $\mathbf{u}_{\text{pore}}$ is the pore velocity. Instead using the Darcy velocity $\mathbf{u}=\mathbf{u}_{\text{pore}}/\varepsilon_{\text{p}}$, multiplying the equation with the porosity ε_{p}, and rescaling γ such that it again can be set proportional to the maximum magnitude of the velocity field $\mathbf{u}$, the equation can be rewritten as:

$$\varepsilon_{\text{p}}\frac{\partial\phi}{\partial t} + \mathbf{u} \cdot \nabla\phi = \gamma\nabla \cdot \left(\varepsilon_{\text{ls}}\nabla\phi - \phi(1-\phi)\frac{\nabla\phi}{|\nabla\phi|}\right) \tag{5-6}$$

This is the nonconservative form of the level set equation that is solved in the Porous Medium feature.

To obtain exact numerical conservation of the integral of $\varepsilon_{\text{p}}\phi$, switch to the conservative form

$$\frac{\partial}{\partial t}(\varepsilon_{\text{p}}\phi) + \nabla \cdot (\mathbf{u}\phi) = \gamma\nabla \cdot \left(\varepsilon_{\text{ls}}\nabla\phi - \phi(1-\phi)\frac{\nabla\phi}{|\nabla\phi|}\right) \tag{5-7}$$

The conservative form can be derived from the nonconservative form if it is assumed that the velocity field $\mathbf{u}$ satisfies the following continuity equation:

$$\frac{\partial\varepsilon_{\text{p}}}{\partial t} + \nabla \cdot \mathbf{u} = 0 \tag{5-8}$$

Initializing the Level Set Function

If the study type Transient with Phase Initialization is used in the model, the level set variable is first initialized so that it varies smoothly between zero and one over the interface. For that study, two study steps are created, Phase Initialization and Time Dependent. The Phase Initialization step solves for the distance to the initial interface, D_{wi}. The Time Dependent step then uses the initial condition for the level set function according to the following expression:

$$\phi_0 = \frac{1}{1 + e^{-D_{\text{wi}}/\varepsilon}}$$

in domains initially outside the interface and

$$\phi_0 = \frac{1}{1 + e^{D_{wi}/\varepsilon}}$$

in domains initially inside the interface. Here, inside refers to domains where $\phi < 0.5$ and outside refers to domains where $\phi > 0.5$.

!	If the **Transient with Phase Initialization** ( ) study is being used, then, for the initialization to work, it is crucial that there are two **Initial Values** nodes. One of the Initial Values nodes should use **Specify phase: Fluid 1 ($\phi = 0$)** and the other **Specify phase: Fluid 2 ($\phi = 1$)**. The initial fluid-fluid interface is then automatically placed on all interior boundaries between both phases. The smooth initialization is not used in domains with **User defined** initial values.

	• The Level Set Interface • Studies and Solvers and Time Dependent with Initialization in the *COMSOL Multiphysics Reference Manual*

Variables For Geometric Properties of the Interface

Geometric properties of the interface are often needed. The unit normal to the interface is given by

$$\mathbf{n} = \left.\frac{\nabla\phi}{|\nabla\phi|}\right|_{\phi = 0,5} \tag{5-9}$$

This variable is available in the physics interface as the interface normal `ls.intnorm`.

Reference for the Level Set Interface

1. E. Olsson and G. Kreiss, “A Conservative Level Set Method for Two Phase Flow,” *J. Comput. Phys.*, vol. 210, pp. 225–246, 2005.

Theory for the Phase Field in Fluids Interface

The Phase Field in Fluids Interface theory is described in this section:

- About the Phase Field Method
- The Equations for the Phase Field Method
- Conservative and Nonconservative Forms
- Additional Sources of Free Energy
- Initializing the Phase Field Function
- Variables and Expressions
- Reference for the Phase Field in Fluids Interface

About the Phase Field Method

The phase field method offers an attractive alternative to more established methods for solving multiphase flow problems. Instead of directly tracking the interface between two fluids, the interfacial layer is governed by a phase field variable, ϕ. The surface tension force is added to the Navier–Stokes equations as a body force by multiplying the chemical potential of the system by the gradient of the phase field variable.

The evolution of the phase field variable is governed by the *Cahn–Hilliard equation*, which is a 4th-order PDE. The Phase Field in Fluids interface decomposes the Cahn–Hilliard equation into two second-order PDEs.

For the level set method, the fluid interface is simply advected with the flow field. The Cahn–Hilliard equation, on the other hand, does not only convect the fluid interface, but it also ensures that the total energy of the system diminishes correctly. The phase field method thus includes more physics than the level set method.

The free energy of a system of two immiscible fluids consists of mixing, bulk distortion, and anchoring energy. For simple two-phase flows, only the mixing energy is retained, which results in a rather simple expression for the free energy.

The Equations for the Phase Field Method

The free energy is a functional of a dimensionless phase field parameter, ϕ:

$$F(\phi, \nabla\phi, T) = \int\left(\frac{1}{2}\varepsilon^2|\nabla\phi|^2 + f(\phi, T)\right)dV = \int f_{\text{tot}}dV$$

where ε is a measure of the interface thickness. Equation 5-10 describes the evolution of the phase field parameter:

$$\frac{\partial\phi}{\partial t} + (\mathbf{u}\cdot\nabla)\phi = \nabla\cdot\gamma\nabla\left(\frac{\partial f_{\text{tot}}}{\partial\phi} - \nabla\cdot\frac{\partial f_{\text{tot}}}{\partial\nabla\phi}\right) \tag{5-10}$$

where f_{tot} (SI unit: J/m^3) is the total free energy density of the system, and $\mathbf{u}$ (SI unit: m/s) is the velocity field for the advection. The right-hand side of Equation 5-10 aims to minimize the total free energy with a relaxation time controlled by the mobility γ (SI unit: $\text{m}^3\cdot\text{s/kg}$).

The free energy density of an isothermal mixture of two immiscible fluids is the sum of the mixing energy and elastic energy. The mixing energy assumes the Ginzburg–Landau form:

$$f_{\text{mix}}(\phi, \nabla\phi) = \frac{1}{2}\lambda|\nabla\phi|^2 + \frac{\lambda}{4\varepsilon^2}(\phi^2 - 1)^2$$

where ϕ is the dimensionless phase field variable, defined such that the volume fraction of the components of the fluid are $(1+\phi)/2$ and $(1-\phi)/2$. The quantity λ (SI unit: N) is the mixing energy density and ε (SI unit: m) is a capillary width that scales with the thickness of the interface. These two parameters are related to the surface tension coefficient, σ (SI unit: N/m), through the equation

$$\sigma = \frac{2\sqrt{2}}{3}\frac{\lambda}{\varepsilon} \tag{5-11}$$

The PDE governing the phase field variable is the Cahn–Hilliard equation:

$$\frac{\partial\phi}{\partial t} + \mathbf{u}\cdot\nabla\phi = \nabla\cdot\gamma\nabla G \tag{5-12}$$

where G (SI unit: Pa) is the chemical potential and γ (SI unit: $\text{m}^3\cdot\text{s/kg}$) is the mobility. The mobility determines the time scale of the Cahn–Hilliard diffusion and must be large enough to retain a constant interfacial thickness but small enough so that the convective terms are not overly damped. In COMSOL Multiphysics the mobility is determined by a mobility tuning parameter that is a function of the interface thickness $\gamma = \chi\varepsilon^2$. The chemical potential is:

$$G = \lambda\left[-\nabla^2\phi + \frac{\phi(\phi^2 - 1)}{\varepsilon^2}\right] \tag{5-13}$$

The Cahn–Hilliard equation forces ϕ to take a value of 1 or −1 except in a very thin region on the fluid-fluid interface. The Phase Field in Fluids interface breaks Equation 5-12 up into two second-order PDEs:

$$\frac{\partial\phi}{\partial t} + \mathbf{u}\cdot\nabla\phi = \nabla\cdot\frac{\gamma\lambda}{\varepsilon^2}\nabla\psi \tag{5-14}$$

$$\psi = -\nabla\cdot\varepsilon^2\nabla\phi + (\phi^2 - 1)\phi \tag{5-15}$$

Conservative and Nonconservative Forms

If the velocity field is divergence free, that is, if

$$\nabla\cdot\mathbf{u} = 0 \tag{5-16}$$

the volume (area for 2D problems) bounded by the interface should be conserved if there is no inflow or outflow through the boundaries. To obtain exact numerical conservation in cases where Equation 5-16 is not fully satisfied, switch to the conservative form

$$\frac{\partial\phi}{\partial t} + \nabla\cdot\mathbf{u}\phi = \nabla\cdot\frac{\gamma\lambda}{\varepsilon^2}\nabla\psi$$

Using the conservative phase field form, exact numerical conservation of the integral of ϕ is obtained. However, the nonconservative form is better suited for numerical calculations and usually converges more easily. The nonconservative form, which is the default form, only conserves the integral of the phase field function approximately, but this is sufficient for most applications.

When the Phase Field in Fluids interface is coupled to a fluid flow interface by means of The Two-Phase Flow, Phase Field Coupling Feature, conservation of the integral of ϕ using the nonconservative form can be improved provided that the discretization order of the phase field variables is equal to or lower than the order of the pressure.

Additional Sources of Free Energy

In some cases, the expression for the free energy can include other sources. It is possible to incorporate these by modifying Equation 5-15:

$$\psi = -\nabla \cdot \varepsilon^2 \nabla\phi + (\phi^2 - 1)\phi + \left(\frac{\varepsilon^2}{\lambda}\right)\frac{\partial f}{\partial \phi} \tag{5-17}$$

where f is a user-defined free energy (SI unit: $\mathrm{J/m^3}$).

	The expression for the external free energy must be manually differentiated with respect to ϕ and then entered into the $\partial f/\partial\phi$ field. In most cases, the external free energy is zero.

Initializing the Phase Field Function

If the study type Transient with Phase Initialization is used in the model, the phase field variable is first initialized so that it varies smoothly between zero and one over the interface. For this study, two study steps are created, Phase Initialization and Time Dependent. The Phase Initialization step solves for the distance to the initial interface, D_{wi}. The Time Dependent step then uses the initial condition for the phase field function according to the expression

$$\phi_0 = -\tanh\left(\frac{D_{\mathrm{wi}}}{\sqrt{2}\varepsilon}\right)$$

in Fluid 1 and

$$\phi_0 = \tanh\left(\frac{D_{\mathrm{wi}}}{\sqrt{2}\varepsilon}\right)$$

in Fluid 2. These expressions are based on a steady, analytic solution to Equation 5-14 and Equation 5-15 for a straight, nonmoving interface.

!	If the **Transient with Phase Initialization** ( ) study is being used, for the initialization to work it is crucial that there are two **Initial Values** nodes. One of the Initial Values nodes is set to **Specify phase: Fluid 1 ($\phi = -1$)** and the other to **Specify phase: Fluid 2 ($\phi = 1$)**. The initial fluid-fluid interface is then automatically placed on all interior boundaries between both phases. The smooth initialization is not used in domains with **User defined** initial values.

	Studies and Solvers in the *COMSOL Multiphysics Reference Manual*

Variables and Expressions

The physics interface defines the chemical potential, which can be rewritten in terms of the dependent variable ψ,

$$G = \frac{\lambda\psi}{\varepsilon^2}$$

and the surface tension force $\mathbf{F} = G\nabla\phi$.

Geometric properties of the interface are often needed. The unit normal to the interface is given by

$$\mathbf{n} = \left.\frac{\nabla\phi}{|\nabla\phi|}\right|_{\phi = 0,5} \tag{5-18}$$

This variable is available in the physics interface as the interface normal `pf.intnorm`.

The mean curvature (SI unit: 1/m) of the interface can be computed by entering the following expression:

$$\kappa = 2(1+\phi)(1-\phi)\frac{G}{\sigma}$$

Reference for the Phase Field in Fluids Interface

1. P. Yue, C. Zhou, J.J. Feng, C.F. Ollivier-Gooch, and H.H. Hu, "Phase-field Simulations of Interfacial Dynamics in Viscoelastic Fluids Using Finite Elements with Adaptive Meshing," *J. Comp. Phys.*, vol. 219, pp. 47–67, 2006.

Theory for the Ternary Phase Field Interface

The Ternary Phase Field Interface theory is described in this section:

- About the Phase Field Method
- The Equations of the Ternary Phase Field Method
- Reference for the Phase Field in Fluids Interface

About the Phase Field Method

The phase field method offers an attractive alternative to more established methods for solving multiphase flow problems. Instead of directly tracking the interface between two fluids, the separating interface is identified as the region across which the phase field variables of the two adjacent phases varies between its two limiting values. The surface tension force is added to the Navier–Stokes equations as a body force by multiplying the chemical potentials of the phases by the gradient of the corresponding phase field variable.

The evolution of each phase field variable is governed by the *Cahn–Hilliard equation*, which is a 4th-order PDE. The Ternary Phase Field interface decomposes each Cahn–Hilliard equation into two second-order PDEs.

For the level set method, the fluid interface is simply advected with the flow field. The Cahn–Hilliard equation, on the other hand, does not only convect the fluid interface, but it also ensures that the total energy of the system diminishes correctly. The phase field method thus includes more physics than the level set method.

The free energy of a system of immiscible fluids consists of mixing, bulk distortion, and anchoring energy. For simple three-phase flows, only the mixing energy is retained.

The Equations of the Ternary Phase Field Method

The ternary phase field model implemented in COMSOL is based the work of Boyer and co-workers in Ref. 2. The model is designed in order to study the evolution of the three immiscible phases, denoted phase A, phase B, and phase C, respectively. Each phase is represented by a phase field variable ϕ, which takes values between 0 and 1. The phase field variables satisfies the constraint

$$\sum_{i = A, B, C} \phi_i = 0 \tag{5-19}$$

and density of each phase is assumed to be constant. This implies that the phase field variable corresponds directly to the volume fraction of the phase in question.

The free energy of the three phase system is defined as a function of the phase field variables in the manner of:

$$\begin{gathered} F = \sigma_{AB}\phi_A^2\phi_B^2 + \sigma_{AC}\phi_A^2\phi_C^2 + \sigma_{BC}\phi_B^2\phi_C^2 + \\ \phi_A\phi_B\phi_C(\Sigma_A\phi_A + \Sigma_B\phi_B + \Sigma_C\phi_C) + \Lambda\phi_A^2\phi_B^2\phi_C^2 \end{gathered} \tag{5-20}$$

Here the σ_{ij} denotes the surface tension coefficient of the interface separating phase i and j, and the capillary parameters Σ_i are defined as

$$\Sigma_i = \sigma_{ij} + \sigma_{ik} - \sigma_{jk} \tag{5-21}$$

and Λ is a function or parameter specifying the additional free bulk energy. By default Λ is zero. In this case it can be seen that the free energy in Equation 5-20 represents the mixing energy, since only interfaces between two phases (where two phase field variables varies between the limiting values) contributes to the free energy.

The Cahn–Hilliard equations to be solved for each phase $p = A, B, C$ are

$$\begin{gathered} \frac{\partial\phi_i}{\partial t} + \frac{\partial u_j\phi_i}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\frac{M_0}{\Sigma_i}\frac{\partial\eta_i}{\partial x_j}\right) \\ \eta_i = \frac{4\Sigma_T}{\varepsilon}\sum_{j \neq i}\left(\frac{1}{\Sigma_j}\left(\frac{\partial F}{\partial\phi_i} - \frac{\partial F}{\partial\phi_j}\right)\right) - \frac{3}{4}\varepsilon\Sigma_j\frac{\partial}{\partial x_j}\left(\frac{\partial\eta_i}{\partial x_j}\right) \end{gathered} \tag{5-22}$$

It can be noted that the Cahn–Hilliard equation is originally a 4th-order PDE. In COMSOL Multiphysics, that PDE is split up into two second-order PDEs by introducing an additional dependent variable, the generalized potential η, one for each phase. In order to satisfy Equation 5-20, two sets of the equations shown in Equation 5-22 are solved, those for phase A and phase B. The phase field variable, and correspondingly the mass fraction, for fluid C is computed from Equation 5-20.

In Equation 5-22 ε (SI unit: 1/m) is a parameter controlling the interface thickness, M_0 (SI unit: m^3/s) is a molecular mobility parameter, and the parameter Σ_T is defined as

$$\frac{3}{\Sigma_{\mathrm{T}}} = \frac{1}{\Sigma_A} + \frac{1}{\Sigma_B} + \frac{1}{\Sigma_C} \tag{5-23}$$

Reference for the Ternary Phase Field Interface

2. F. Boyer, C. Lapuerta, S. Minjeaud, B. Piar, and M. Quintard, "Cahn–Hilliard/Navier–Stokes model for the simulation of three-phase flows", *Transport in Porous Media*, vol. 28, pp. 463–484, 2010.

3. J. J. Jasper, "The Surface Tension of Pure Liquid Compounds", *J. Phys. Chem. Ref. Data.*, vol. 1, no. 4, pp. 841-1009, 1972.

4. R. C. Weast, ed.,"CRC Handbook of Chemistry and Physics", ed. 69, MIT Press, 1988.

5. A. G. Gaonkar, "Interfacial Tensions of Vegetable Oil/Water Systems: Effect of Oil Purification", *J. Am. Oil Chem. Soc.*, vol. 66, no. 8, pp. 1090-1092, 1989.

6

Porous Media Flow Interfaces

This chapter discusses the physics interfaces found under the **Fluid Flow** > **Porous Media and Subsurface Flow** branch ( ). See Modeling Microfluidic Fluid Flows to help you select which physics interface to use.

In this chapter:

- The Darcy's Law Interface
- The Brinkman Equations Interface
- The Free and Porous Media Flow, Brinkman Interface
- The Free and Porous Media Flow, Darcy Interface
- Theory for the Darcy's Law Interface
- Theory for the Brinkman Equations Interface
- Theory for the Free and Porous Media Flow, Brinkman Interface
- Theory for the Free and Porous Media Flow, Darcy Interface

The Darcy's Law Interface

The **Darcy's Law (dl)** interface ( ), found under the **Porous Media and Subsurface Flow** branch ( ) when adding a physics interface, is used to simulate fluid flow through interstices in a porous medium. It can be used to model low-velocity flows or media where the permeability and porosity are very small, and for which the pressure gradient is the major driving force and the flow is mostly influenced by the frictional resistance within the pores. Set up multiple **Darcy's Law** interfaces to model multiphase flows involving more than one mobile phase. The Darcy's Law interface can be used for stationary and time-dependent analyses.

The main feature is the **Porous Medium** Properties node, which provides interfaces for defining the fluid material and the porous matrix properties.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Porous Medium**, **No Flow** (the default boundary condition), and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and mass sources. You can also right-click **Darcy's Law** to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `dl`.

PHYSICAL MODEL

Enter a **Reference pressure level** p_{ref} (SI unit: Pa). The default value is `1[atm]`.

GRAVITY EFFECTS

By default there are no gravity effects added to Darcy's Law interface. Select the checkbox **Include gravity** to activate the acceleration of gravity. When this checkbox is selected, a global **Gravity** feature node is shown in the interface model tree.

Enter a value for the acceleration of gravity. The default value `g_const` is the predefined standard acceleration of gravity on earth.

	For a detailed overview of the functionality available in each product, visit https://www.comsol.com/products/specifications/.

DISCRETIZATION

To display all settings available in this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog.

You can choose the order of the shape functions used for the pressure variable solved by the Darcy's Law interface. The default shape functions are **Quadratic** Lagrange.

The **Compute boundary fluxes** checkbox is not activated by default. When this option is selected, the solver computes variables storing accurate boundary fluxes from each boundary into the adjacent domain.

If the checkbox is cleared, the COMSOL Multiphysics software instead computes the flux variables from the dependent variables using extrapolation, which is less accurate in postprocessing results but does not create extra dependent variables on the boundaries for the fluxes.

Also, the **Apply smoothing to boundary fluxes** checkbox is available if the previous checkbox is checked. The smoothing can provide a better behaved flux value close to singularities.

For details about the boundary fluxes settings, see Computing Accurate Fluxes in the *COMSOL Multiphysics Reference Manual*.

The **Value type when using splitting of complex variables** setting should in most pure mass transport problems be set to **Real** which is the default. It makes sure that the dependent variable does not get affected by small imaginary contributions, which can occur, for example, when combining a Time Dependent or Stationary study with a frequency-domain study. For more information, see Splitting Complex-Valued Variables in the *COMSOL Multiphysics Reference Manual*.

DEPENDENT VARIABLES

The dependent variable (field variable) is the **Pressure**. The name can be changed but the names of fields and dependent variables must be unique within a model.

	• Domain, Boundary, Edge, Point, and Pair Nodes for the Darcy's Law Interface • Theory for the Darcy's Law Interface • Physical Constants in the *COMSOL Multiphysics Reference Manual*

	• *Species Transport in the Gas Diffusion Layers of a PEM*: Application Library path **Fuel_Cell_and_Electrolyzer_Module/Fuel_Cells/pem_gdl_species_transport_2d** • *Steam Reformer*: Application Library path **Chemical_Reaction_Engineering_Module/Reactors_with_Porous_Catalysts/steam_reformer** • *Terzaghi Compaction*: Application Library path **Subsurface_Flow_Module/Poromechanics/terzaghi_compaction**

Domain, Boundary, Edge, Point, and Pair Nodes for the Darcy's Law Interface

The Darcy's Law Interface has the following domain, boundary, edge, point, and pair nodes, these nodes are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

DOMAIN

- Porous Medium
- Unsaturated Porous Medium
- Dual Porosity Medium
- Dual Permeability Medium
- Unsaturated Dual Permeability Medium
- Mass Source
- Cross Section
- Initial Values
- Unsaturated Porous Medium
- ThicknessContributing Velocity
- Porous Electrode Coupling

BOUNDARY, EDGE, AND POINT

The following nodes (listed in alphabetical order) are available on exterior boundaries:

- Atmosphere/Gauge
- Electrode Surface Coupling
- Flux Discontinuity
- Fracture
- Hydraulic Head
- Inlet
- Interior Wall
- Line Mass Source
- Mass Flux
- No Flow
- Outlet
- Pervious Layer
- Point Mass Source
- Precipitation
- Pressure
- Pressure Head
- [1]
- Symmetry
- Thin Barrier

[1] This node is described for the Transport of Diluted Species Interface

The relevant physics interface condition at interior boundaries is continuity:

$$\mathbf{n} \cdot (\rho_1 \mathbf{u}_1 - \rho_2 \mathbf{u}_2) = 0$$

The continuity boundary condition ensures that the pressure and mass flux are continuous. In addition, the Pressure boundary condition is available on interior boundaries.

The continuity boundary condition provides continuity for the pressure and mass flux. In addition, the following boundary conditions are available on interior boundaries:

- Pressure
- Pressure Head
- Hydraulic Head
- Interior Wall
- Pervious Layer
- Flux Discontinuity
- Fracture
- Thin Barrier

	Note that some of the above-mentioned domain or boundary conditions are only available with some products. For a detailed overview of the functionality available in each product, visit https://www.comsol.com/products/specifications/

	In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

	For axisymmetric components, COMSOL Multiphysics takes the axial symmetry boundaries (at $r = 0$) into account and automatically adds an **Axial Symmetry** node that is valid on the axial symmetry boundaries only.

	In the *COMSOL Multiphysics Reference Manual* see Table 2-4 for links to common sections and Table 2-5 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Porous Medium

The **Porous Medium** node adds the equations for modeling flow through porous domains. By default these are Equation 6-1 and Equation 6-2 (excluding any mass sources).

$$\frac{\partial}{\partial t}(\varepsilon_p \rho) + \nabla \cdot (\rho \mathbf{u}) = Q_{\mathrm{m}} \tag{6-1}$$

$$\mathbf{u} = -\frac{\kappa}{\mu}\nabla p \tag{6-2}$$

For a steady-state problem the first term in Equation 6-1 disappears. When Mass Source is active Equation 6-2 is of the following form:

$$\mathbf{u} = -\frac{\kappa}{\mu}(\nabla p - \rho \mathbf{g}) \tag{6-3}$$

The **Porous Medium** feature has two default subfeatures — the Fluid subfeature where the fluid density ρ (SI unit: kg/m^3) and dynamic viscosity μ (SI unit: Pa·s) are defined and the Porous Matrix subfeature where the permeability κ (SI unit: m^2) and porosity ε_p (dimensionless) are specified.

COORDINATE SYSTEM SELECTION

Select a coordinate system from the **Coordinate system** list for the interpretation of directions in anisotropic material properties. The default is the **Global coordinate system**, and the list contains any additional orthonormal coordinate system (except boundary coordinate systems) added under the **Definitions** node.

The subnodes inherit these coordinate system settings. In particular, the **Permeability** or **Hydraulic conductivity** (in the Porous Matrix subnode) should be set according to the coordinate system selected in this section.

FLOW MODEL

Define if the flow follows a linear or nonlinear pressure-velocity relationship.

- **Darcian flow** (default) defines a linear relationship using Equation 6-1 and Equation 6-2.
- **Non-Darcian flow** defines a nonlinear relationship using Equation 6-1 and

$$\nabla p = -\frac{\mu}{\kappa}\mathbf{u} - \beta\rho|\mathbf{u}|\mathbf{u}$$

  where the nonlinear parameter β (SI unit: $1/m$) is further specified in the Porous Matrix subfeature.

STORAGE MODEL

Define the time dependent storage term by selecting one of the following options from the list:

- **From density and porosity** (default), uses the formulation of Equation 6-1

- **Linearized storage**, where the following linear equation is used to define the storage:

$$S_p = \varepsilon_p \chi_f + (1 - \varepsilon_p)\chi_p$$

- **Poroelastic storage**, where $S_p = \varepsilon_p \chi_f$
- **Quasistatic**, where the storage term is set to zero
- **User defined** to directly specify the storage coefficient S_p

	• Porous Material in the *COMSOL Multiphysics Reference Manual* • About Darcian and Non-Darcian Flow in the *Porous Media Flow Module User's Guide* • Storage Models in the *Subsurface Flow Module User's Guide*

	Note that some options are only available in some modules. For a detailed overview of the functionality available in each product, visit https://www.comsol.com/products/specifications/

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Porous Medium**

Richards' Equation > **Porous Medium**

Ribbon

Physics tab with *interface* as **Darcy's Law** or **Richards' Equation** selected:

Domains > *interface* > **Porous Medium**

Fluid

This node defines the material properties of the fluid of the Porous Medium, the Unsaturated Porous Medium, the Dual Porosity Medium, the Dual Permeability Medium, or the Unsaturated Porous Medium parent node.

MODEL INPUT

This section contains fields and values that are inputs for expressions defining material properties. If such user-defined property groups are added, the model inputs appear here.

FLUID PROPERTIES

The available options for the **Fluid type** are **Incompressible**, **Compressible**, **Compressible, linearized**, or **Ideal gas**. The selection determines how the density and compressibility of the fluid are set.

Incompressible

The default **Reference density** ρ_{ref} uses values **From material**. For **User defined** enter another value or expression.

Compressible

The default **Density** ρ uses values **From material**. For **User defined** enter another value or expression as a function of the absolute pressure. The compressibility of the fluid is computed from it.

Compressible, Linearized

The default **Reference density** ρ_{ref} and the **Fluid compressibility** χ_{f} use values **From material**. For **User defined** enter another value or expression. The fluid density increases linearly as a function of the fluid pressure.

Ideal Gas

For **Ideal gas** it uses the ideal gas law to describe the gas density. In this case, specify the thermodynamics properties. Select a **Gas constant type** — **Specific gas constant** R_s (the default) or **Mean molar mass** M_n (SI unit: J/(mol·K)). For **Mean molar mass** the universal gas constant $R = 8.314$ J/(mol·K) is used as the built-in physical constant. For both properties, the defaults use values **From material**. For **User defined** enter another value or expression.

Dynamic Viscosity

For all fluid types specify the **Dynamic viscosity** μ (SI unit: Pa·s) uses values **From material**. For **User defined** enter another value or expression.

Constitutive Relation

The Polymer Flow Module allows the use of inelastic non-Newtonian models. For Darcian Flow, you can choose between two options: **Specify dynamic viscosity** (default) or **Inelastic non-Newtonian**. Use the default option to either get the dynamic viscosity from a material, or to add a user defined expression. The default option lets you either use the dynamic viscosity from a material or define it with a custom expression. The **Inelastic non-Newtonian** option provides several models and defines the **Apparent shear rate**.

Inelastic Non-Newtonian

The following inelastic non-Newtonian Models are available for the **Fluid** feature under the **Porous Medium** feature:

- Power Law
- Carreau
- Carreau-Yasuda
- Cross
- Cross-Williamson
- Sisko

The setup of these models in porous media is similar to their definition under the Fluid Properties feature.

Apparent Shear Rate

To define the apparent shear rate $\dot{\gamma}_{\text{app}}$, either enter a user-defined expression for the correction factor (α) or choose the **Capillary bundle approach** from the list and provide a value for the Tortuosity factor (C).

	• Read more about the theory of Non-Newtonian Fluids in Porous Media in the *Polymer Flow Module User's Guide*

LOCATION IN USER INTERFACE

A default **Fluid** node is automatically added to the Porous Medium, the Unsaturated Porous Medium, the Dual Porosity Medium, the Dual Permeability Medium, and the Unsaturated Dual Permeability Medium node.

Context Menus

Darcy's Law > *porous medium feature* > **Fluid**
Richards' Equation > *porous medium feature* > **Fluid**

Porous Matrix

This node defines the porosity and material properties of the solid matrix of the Porous Medium or Unsaturated Porous Medium parent node.

MODEL INPUT

This section contains fields and values that are inputs for expressions defining material properties. If such user-defined property groups are added, the model inputs appear here.

MATRIX PROPERTIES

The default **Porosity** ε_p of the solid matrix is taken **From material**. In a **Porous Material** node, the porosity is defined as follows:

$$\varepsilon_p = 1 - \sum_i \theta_{si} - \sum_i \theta_{imfi}$$

where θ_{si} and θ_{imfi} are the porosities of the **Solid** and **Immobile Fluids** subnodes under the **Porous Material** node. See Porous Material in the *COMSOL Multiphysics Reference Manual* for more information.

Select **User defined** to enter a value or expression for ε_p.

If required by a **Storage model** in the parent node, specify the **Effective compressibility** of the porous matrix. The default value is $\chi_p = 10^{-4}$ 1/Pa.

Select a **Permeability model** to specify the capacity of the porous material to transmit flow. Which options are available depends on the **Flow model** setting in the parent node. Note that for the Unsaturated Porous Medium parent node only the Darcian Flow models are available.

Darcian Flow

If **Darcian flow** is selected in the parent **Porous medium** node, select between the following options for the **Permeability model**:

- Select **Permeability** (default) to define the permeability of the porous matrix. The default **Permeability** κ (SI unit: m^2) uses the value **From material**, as defined by the **Porous material**. For **User defined** select **Isotropic** to define a scalar value or **Diagonal** or **Symmetric** to define a tensor value.
- Select **Hydraulic conductivity** or define a combination of fluid permeability and dynamic viscosity. For **Hydraulic conductivity** K (SI unit: m/s) select **Isotropic** to define a scalar value or **Diagonal** or **Symmetric** to define a tensor value. The default is $2.94 \cdot 10^{-4}$ m/s.
- Select **Kozeny-Carman** to define the permeability from the porosity and mean particle diameter. Enter the mean **Particle diameter** d_p (SI unit: m), the default value is 0.5 mm.

Non-Darcian Flow

If **Non-Darcian flow** is selected in the parent node, select between the following options for the **Permeability model**:

- For **Forchheimer**, the default **Permeability** κ (SI unit: m^2) uses the value **From material**. Furthermore, the dimensionless **Forchheimer parameter** c_F can be defined. The default value is 0.55.
- If **Ergun** is selected, enter the mean **Particle diameter** d_p (default value: 0.5 mm).
- For **Burke–Plummer**, specify the mean **Particle diameter** d_p (default value: 0.5 mm).
- For **Klinkenberg**, the default **Permeability** κ_∞ (SI unit: m^2) uses the value **From material**. Enter the **Klinkenberg parameter** b_K. Its default value is 10^3 Pa.

	• About Darcian and Non-Darcian Flow in the *Porous Media Flow Module User's Guide* • Permeability Models in the *Porous Media Flow Module User's Guide*

	Note that some options are only available in some modules. For a detailed overview of the functionality available in each product, visit https://www.comsol.com/products/specifications/

RETENTION MODEL

For an Unsaturated Porous Medium select between the following options for the retention model:

- **van Genuchten**, to specify the retention model using the van Genuchten relationship. Enter the constitutive relation constants α (the default value is 1, and the SI unit is 1/m), n (default value is 2), and l (default value is 0.5). The constitutive parameter m is equal to $1 - 1/n$.
- **Brooks and Corey** to use the retention model according to the Brooks and Corey relationships.
- **User defined** to use a different retention model. Enter user defined expressions for the **Effective saturation** S_e, the **Liquid volume fraction** θ_l. The default is ε_p (the porosity variable). Specify the **Specific moisture capacity** C_m (SI unit: 1/m). The default value is 0 (1/m). Enter an expression for the **Relative permeability** κ_r. The default value is 1.

If there is a residual volume of liquid that cannot move through the pore network, also enter a value between 0 and 1 for the **Residual liquid volume fraction** θ_r. The default value is 0.

	Retention and Permeability Relationships in the *Subsurface Flow Module User's Guide*

LOCATION IN USER INTERFACE

A default **Porous Matrix** node is automatically added to Porous Medium or the Unsaturated Porous Medium node.

Context Menus

Darcy's Law > *porous medium feature* > **Fluid**

Richards' Equation > *porous medium feature* > **Fluid**

Unsaturated Porous Medium

The **Unsaturated Porous Medium** node adds Richards' equation (Equation 6-4) for flow in variably saturated porous media.

$$\rho\left(\frac{C_m}{\rho g} + S_e S_p\right)\frac{\partial p}{\partial t} + \nabla \cdot \rho\left(-\frac{\kappa_r \kappa}{\mu}(\nabla p + \rho g \nabla D)\right) = Q_m \tag{6-4}$$

The Unsaturated Porous Medium feature has two default subfeatures: the Fluid subfeature, where the fluid density ρ (SI unit: kg/m^3) and viscosity μ (SI unit: Pa·s) are defined, and the Porous Matrix subfeature, where the permeability κ (SI unit: m^2) and porosity ε_p (dimensionless) are specified as well as the retention model.

COORDINATE SYSTEM SELECTION

Select a coordinate system from the **Coordinate system** list for the interpretation of directions in anisotropic material properties. The default is the **Global coordinate system**, and the list contains any additional orthonormal coordinate system (except boundary coordinate systems) added under the **Definitions** node.

The subnodes inherit these coordinate system settings. In particular, the **Permeability** or **Hydraulic conductivity** (in the Porous Matrix subnode) should be set according to the coordinate system selected in this section.

STORAGE MODEL

With this option, define the first term in Equation 6-4. Therefore, choose from a list one of the following formulations:

- From retention model
- Linearized storage (default)
- From liquid content
- User defined

If **From retention model** is chosen, the first term of Equation 6-4 accounts only for the specific moisture capacity C_m which is defined by the Retention Model in the Porous Matrix subnode:

$$\frac{C_m}{g}\frac{\partial p}{\partial t}.$$

For the option **Linearized storage** the storage coefficient S_p in Equation 6-4 is defined as

$$S_p = \varepsilon_p \chi_f + (1 - \varepsilon_p)\chi_p .$$

From liquid content enforces the first term of Equation 6-4 to be defined in terms of liquid volume fraction as

$$\frac{\partial(\rho\theta_l)}{\partial t}$$

and the **User defined** option allows to define the storage coefficient S_p in Equation 6-4 directly.

	Note that some options are only available in some modules. For a detailed overview of the functionality available in each product, visit https://www.comsol.com/products/specifications/

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Unsaturated Porous Medium**

Richards' Equation > **Unsaturated Porous Medium**

Ribbon

Physics tab with *interface* as **Darcy's Law** or **Richards' Equation** selected:

Domains > *interface* > **Unsaturated Porous Medium**

Dual Porosity Medium

Use the Dual Porosity Medium if the flow through macropores is governed by Darcy's law and the micropores do not significantly contribute to the overall flow in the porous medium.

The feature has three default subfeatures —the Fluid subfeature where the fluid density ρ (SI unit: kg/m^3) and dynamic viscosity μ (SI unit: Pa·s) are defined, the Macropores subfeature where the hydraulic properties of the macroporous matrix are defined, and the Micropores where the hydraulic properties of the microporous matrix are defined.

COORDINATE SYSTEM SELECTION

Select a coordinate system from the **Coordinate system** list for the interpretation of directions in anisotropic material properties. The default is the **Global coordinate system**, and the list contains any additional orthonormal coordinate system (except boundary coordinate systems) added under the **Definitions** node.

The subnodes inherit these coordinate system settings. In particular, the **Permeability** or **Hydraulic conductivity** (in the Macropores and Micropores subnodes) should be set according to the coordinate system selected in this section.

STORAGE MODEL

Choose from a list one of the following formulations:

- **From density and porosity** (default), uses the formulation equivalent to Equation 6-1
- **Linearized storage**, where the following linear equation is used to define the storage in the macropores as $S_p = \varepsilon_p\chi_f + (1 - \varepsilon_p)\chi_p$ and in the micropores as $S_{p,m} = \varepsilon_{p,m}\chi_f + (1 - \varepsilon_{p,m})\chi_p$.
- **Poroelastic storage**, where $S_p = \varepsilon_p\chi_f$ in the macropores and $S_{p,m} = \varepsilon_{p,m}\chi_f$ in the micropores.

- **Quasistatic**, where the storage term is set to zero
- **User defined** to directly specify the storage coefficient S_p and $S_{p,m}$ for the macro- and micropores respectively.

	• Storage Models in the *Subsurface Flow Module User's Guide*

INTERPOROSITY FLOW

Specify the **Fluid Transfer Function** α_w which is used to calculate the interporosity flow, the mass exchange between macro- and microscale system:

$$Q_{ip} = \alpha_w(p_M - p_m) \tag{6-5}$$

with p_M being the pressure within the macropores and p_m the pressure within the micropores.

	Find more information in the *Subsurface Flow Module User's Guide* • Dual Porosity & Dual Permeability Modeling • Dual Porosity and Dual Permeability Theory

	Note that some options are only available in some modules. For a detailed overview of the functionality available in each product, visit https://www.comsol.com/products/specifications/

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Dual Porosity/Permeability** > **Dual Porosity Medium**

Richards' Equation > **Dual Porosity/Permeability** > **Dual Porosity Medium**

Ribbon

Physics tab with **Darcy's Law** or **Richards' Equation** selected:

Domains > **Dual Porosity/Permeability** > **Dual Porosity Medium**

Dual Permeability Medium

Use the **Dual Permeability Medium** feature to model transport in a saturated dual permeability medium where Darcy's Law describes the transport in each system.

The feature has three default subfeatures —the Fluid subfeature where the fluid density ρ (SI unit: kg/m^3) and dynamic viscosity μ (SI unit: Pa·s) are defined, the Macropores subfeature where the hydraulic properties of the macroporous matrix are defined, and the Micropores where the hydraulic properties of the microporous matrix are defined.

COORDINATE SYSTEM SELECTION

Select a coordinate system from the **Coordinate system** list for the interpretation of directions in anisotropic material properties. The default is the **Global coordinate system**, and the list contains any additional orthonormal coordinate system (except boundary coordinate systems) added under the **Definitions** node.

The subnodes inherit these coordinate system settings. In particular, the **Permeability** or **Hydraulic conductivity** (in the Macropores and Micropores subnodes) should be set according to the coordinate system selected in this section.

STORAGE MODEL

With this option under the **Porous Medium** section, Equation 6-1 is formulated with respect to a storage term (analogous to Equation 4-4). Therefore, choose from a list one of the following formulations:

- **From density and porosity** (default), uses the formulation of Equation 4-4
- **Linearized storage**, where the following linear equation is used to define the storage:

$$S_{p,i} = \varepsilon_{p,i}\chi_f + (1 - \varepsilon_{p,i})\chi_{p,i}$$

with i=M for the macropores and i=m for the micropores.

- **Poroelastic storage**, where $S_{p,i} = \varepsilon_{p,i}\chi_f$
- **Quasistatic**, where the storage term is set to zero
- **User defined** to directly specify the storage coefficient S_p

- Storage Models in the *Subsurface Flow Module User's Guide*

INTERPOROSITY FLOW

Specify the **Fluid Transfer Function** α_w which is used to calculate the interporosity flow, which is the mass exchange between macro- and microscale system:

$$Q_{ip} = \alpha_w(p_M - p_m) \tag{6-6}$$

with p_M being the pressure in the macropores and p_m the pressure in the micropores.

	Find more information in the *Subsurface Flow Module User's Guide* • Dual Porosity & Dual Permeability Modeling • Dual Porosity and Dual Permeability Theory

	Note that some options are only available in some modules. For a detailed overview of the functionality available in each product, visit https://www.comsol.com/products/specifications/

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Dual Porosity/Permeability** > **Dual Permeability Medium**
Richards' Equation > **Dual Porosity/Permeability** > **Dual Permeability Medium**

Ribbon

Physics tab with **Darcy's Law** or **Richards' Equation** selected:

Domains > **Dual Porosity/Permeability** > **Dual Permeability Medium**

Unsaturated Dual Permeability Medium

Use the **Unsaturated Dual Permeability Medium** feature to model the transport in an unsaturated dual permeability medium where Richards' Equation (Equation 6-4) describes the transport in each system.

$$\begin{gathered}
\theta_M\left(\rho\left(S_{e,M}S_{p,M} + \frac{C_{m,M}}{\rho g}\right)\frac{\partial p_M}{\partial t} + \nabla(\rho \mathbf{u}_M)\right) = -Q_{ip} + \theta_M Q_m \\
(1-\theta_M)\left(\rho\left(S_{e,m}S_{p,m} + \frac{C_{m,m}}{\rho g}\right)\frac{\partial p_m}{\partial t} + \nabla(\rho \mathbf{u}_m)\right) = Q_{ip} + (1-\theta_M)Q_m \\
p = \theta_M p_M + (1-\theta_M)p_m
\end{gathered} \tag{6-7}$$

θ_M is the volume fraction of the macropores and Q_{ip} is the interporosity flow, which is the mass transfer from the macroscale to the microscale system. The indices M and m stand for macropores and micropores, respectively.

The feature has three default subfeatures —the Fluid subfeature where the fluid density ρ (SI unit: kg/m^3) and dynamic viscosity μ (SI unit: Pa·s) are defined, the Macropores subfeature where the hydraulic properties of the macroporous matrix are defined, and the Micropores where the hydraulic properties of the microporous matrix are defined.

COORDINATE SYSTEM SELECTION

Select a coordinate system from the **Coordinate system** list for the interpretation of directions in anisotropic material properties. The default is the **Global coordinate system**, and the list contains any additional orthonormal coordinate system (except boundary coordinate systems) added under the **Definitions** node.

The subnodes inherit these coordinate system settings. In particular, the **Permeability** or **Hydraulic conductivity** (in the Macropores and Micropores subnodes) should be set according to the coordinate system selected in this section.

STORAGE MODEL

With this option, define the first term in Equation 6-7. Therefore, choose from a list one of the following formulations:

- From retention model
- Linearized storage (default)
- From liquid content
- User defined

If **From retention model** is chosen, the first term of Equation 6-7 accounts only for the specific moisture capacity $C_{m,i}$ which is defined by the Retention Model in the Macropores (i=M) or Micropores (i=m) subnode:

$$\frac{C_{\mathrm{m}i}}{g}\frac{\partial p}{\partial t}.$$

For the option **Linearized storage** the storage coefficient $S_{p,i}$ in Equation 6-7 is defined as

$$S_{p,i} = \varepsilon_{p,i}\chi_f + (1-\varepsilon_{p,i})\chi_{p,i}.$$

From liquid content enforces the first term of Equation 6-7 to be defined in terms of liquid volume fraction as

$$\frac{\partial(\rho\theta_{l,i})}{\partial t}$$

- and the **User defined** option allows to define the storage coefficient $S_{p,i}$ in Equation 6-7 directly.

- Storage Models in the *Subsurface Flow Module User's Guide*

INTERPOROSITY FLOW

Specify the **Fluid Transfer Function** α_w which is used to calculate the interporosity flow, which is the mass exchange between macro- and microscale system:

$$Q_{ip} = \alpha_w(p_M - p_m) \tag{6-8}$$

with p_M being the pressure within the macroscale system and p_m the pressure within the microscale system.

- Dual Porosity & Dual Permeability Modeling in the *Subsurface Flow Module User's Guide*

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Dual Porosity/Permeability** > **Unsaturated Dual Permeability Medium**

Richards' Equation > **Dual Porosity/Permeability** > **Unsaturated Dual Permeability Medium**

Ribbon

Physics tab with **Darcy's Law** or **Richards' Equation** selected:

Domains > **Dual Porosity/Permeability** > **Unsaturated Dual Permeability Medium**

Macropores

This node defines the porosity and material properties of the macroporous matrix of the Dual Porosity Medium, the Dual Permeability Medium, or the Unsaturated Dual Permeability Medium parent node.

MODEL INPUT

This section contains fields and values that are inputs for expressions defining material properties. If such user-defined property groups are added, the model inputs appear here.

VOLUME FRACTION

Here enter the **Volume Fraction of Macropores**, θ_M.

MATRIX PROPERTIES

The default **Porosity** $\varepsilon_{p,M}$ of the solid matrix of the macropore system is taken **From material**. Select **User defined** to enter a value or expression for $\varepsilon_{p,M}$.

If required by a **Storage model** in the parent node, specify the **Effective compressibility** of the porous matrix of the macropore system. The default value is $\chi_{p,M} = 10^{-4}$ 1/Pa.

Select a **Permeability model** to specify the capacity of the porous material to transmit flow. For the macropore settings only the Darcian Flow models are available. Select between the following options for the **Permeability model**:

- Select **Permeability** (default) to define the permeability of the porous matrix. The default **Permeability** κ_M (SI unit: m^2) uses the value **From material**, as defined by the **Porous material**. For **User defined** select **Isotropic** to define a scalar value or **Diagonal** or **Symmetric** to define a tensor value.
- Select **Hydraulic conductivity** or define a combination of fluid permeability and dynamic viscosity. For **Hydraulic conductivity** K_M (SI unit: m/s) select **Isotropic** to define a scalar value or **Diagonal** or **Symmetric** to define a tensor value. The default is $2.94 \cdot 10^{-4}$ m/s.
- Select **Kozeny-Carman** to define the permeability from the porosity and mean particle diameter. Enter the mean **Particle diameter** $d_{p,M}$ (SI unit: m), the default value is 0.5 mm.

RETENTION MODEL

For an Unsaturated Dual Permeability Medium select between the following options for the retention model:

- **van Genuchten**, to specify the retention model using the van Genuchten relationship. Enter the constitutive relation constants α (the default value is 1, and the SI unit is 1/m), n (default value is 2), and l (default value is 0.5). The constitutive parameter m is equal to $1 - 1/n$.

- **Brooks and Corey** to use the retention model according to the Brooks and Corey relationships.
- **User defined** to use a different retention model. Enter user defined expressions for the **Effective saturation** $S_{e,M}$, the **Liquid volume fraction** $\theta_{l,M}$. The default is $\varepsilon_{p,M}$ (the porosity variable). Specify the **Specific moisture capacity** $C_{m,M}$ (SI unit: $1/m$). The default value is 0 ($1/m$). Enter an expression for the **Relative permeability** $\kappa_{r,M}$. The default value is 1.

If there is a residual volume of liquid that cannot move through the pore network, also enter a value between 0 and 1 for the **Residual liquid volume fraction** θ_r. The default value is 0.

	Retention and Permeability Relationships in the *Subsurface Flow Module User's Guide*

LOCATION IN USER INTERFACE

A default **Macropores** node is automatically added to the Dual Porosity Medium, the Dual Permeability Medium, and the Unsaturated Dual Permeability Medium node.

Context Menus

Darcy's Law > *porous medium feature* > **Macropores**
Richards' Equation > *porous medium feature* > **Macropores**

Micropores

This node defines the porosity and material properties of the microporous matrix of the Dual Porosity Medium, Dual Permeability Medium, or the Unsaturated Dual Permeability Medium parent node.

MODEL INPUT

This section is only available for the Unsaturated Dual Permeability Medium parent node and contains fields and values that are inputs for expressions defining material properties. If such user-defined property groups are added, the model inputs appear here.

MATRIX PROPERTIES

The default **Porosity** $\varepsilon_{p,m}$ of the solid matrix of the micropore system is taken **From material**. Select **User defined** to enter a value or expression for $\varepsilon_{p,m}$.

If required by a **Storage model** in the parent node, specify the **Effective compressibility** of the microscale porous matrix. The default value is $\chi_{p,m} = 10^{-4}$ 1/Pa.

Select a **Permeability model** to specify the capacity to transmit flow for the porous material of the microscale system. Here, only the Darcian Flow models are available. Select between the following options for the **Permeability model**:

- Select **Permeability** (default) to define the permeability of the porous matrix. The default **Permeability** κ_m (SI unit: m^2) uses the value **From material**, as defined by the **Porous material**. For **User defined** select **Isotropic** to define a scalar value or **Diagonal** or **Symmetric** to define a tensor value.
- Select **Hydraulic conductivity** or define a combination of fluid permeability and dynamic viscosity. For **Hydraulic conductivity** K_m (SI unit: m/s) select **Isotropic** to define a scalar value or **Diagonal** or **Symmetric** to define a tensor value. The default is $2.94 \cdot 10^{-4}$ m/s.
- Select **Kozeny-Carman** to define the permeability from the porosity and mean particle diameter. Enter the mean **Particle diameter** $d_{p,m}$ (SI unit: m), the default value is 0.5 mm.

RETENTION MODEL

For an Unsaturated Dual Permeability Medium select between the following options for the retention model:

- **From macropores** to take over the retention model settings from the **Macropores** node.
- **van Genuchten**, to specify the retention model using the van Genuchten relationship. Enter the constitutive relation constants α (the default value is 1, and the SI unit is 1/m), n (default value is 2), and l (default value is 0.5). The constitutive parameter m is equal to $1 - 1/n$.
- **Brooks and Corey** to use the retention model according to the Brooks and Corey relationships.
- **User defined** to use a different retention model. Enter user defined expressions for the **Effective saturation** $S_{e,m}$, the **Liquid volume fraction** $\theta_{l,m}$. The default is $\varepsilon_{p,m}$ (the porosity variable). Specify the **Specific moisture capacity** $C_{m,m}$ (SI unit: 1/m). The default value is 0 (1/m). Enter an expression for the **Relative permeability** $\kappa_{r,m}$. The default value is 1.

If there is a residual volume of liquid that cannot move through the pore network, also enter a value between 0 and 1 for the **Residual liquid volume fraction** θ_r. The default value is 0.

	Retention and Permeability Relationships in the *Subsurface Flow Module User's Guide*

INITIAL VALUES

Define the initial pressure of the microscale system. The default is to use the initial values defined in the Initial Values feature node which means that the same initial values apply to the macroscale and the microscale system.

Select **User Defined** to specify an initial pressure for the microscale system $p_{m0,init}$.

	Note that some options are only available in some modules. For a detailed overview of the functionality available in each product, visit https://www.comsol.com/products/specifications/

LOCATION IN USER INTERFACE

A default **Micropores** node is automatically added to the Dual Porosity Medium, the Dual Permeability Medium, and the Unsaturated Dual Permeability Medium node.

Context Menus

Darcy's Law > *porous medium feature* > **Micropores**
Richards' Equation > *porous medium feature* > **Micropores**

Mass Source

The **Mass Source** node adds a mass source Q_m, which appears on the right-hand side of the Darcy's Law equation (Equation 6-1).

$$\frac{\partial}{\partial t}(\rho\varepsilon) + \nabla \cdot (\rho \mathbf{u}) = Q_m \tag{6-9}$$

For the Fracture Flow interface, the mass source is applicable to the right-hand side of Equation 4-40 in the *Subsurface Flow Module User's Guide* (where it is multiplied with the fracture thickness).

MASS SOURCE

Enter a value or expression for the **Mass source** Q_m (SI unit: kg/(m^3·s)). The default is 0 kg/(m^3·s).

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Mass Source**

Richards' Equation > **Mass Source**

Ribbon

Physics tab with *interface* as **Darcy's Law** or **Richards' Equation** selected:

Domains > *interface* > **Mass Source**

Contributing Velocity

The **Contributing Velocity** node adds a velocity contribution $\mathbf{u}_{\text{ctrb}}$ to the velocity field $\mathbf{u}_{\text{d}}$ that is computed from the flow model selected in the parent Porous Medium, Unsaturated Porous Medium, or Dual Porosity Medium feature. The total velocity field used in the continuity equation is therefore

$$\mathbf{u} = \mathbf{u}_{\text{d}} + \mathbf{u}_{\text{ctrb}} \tag{6-10}$$

Such velocity contributions can arise in multiphysics models that involve, for example, transport of solutes. If several **Contributing Velocity** nodes are added under the same parent feature, the contributions are treated additively. The sum of all contributing velocity fields is available in the variables `name.Uctrb` (material frame) and `name.uctrb` (spatial frame), with `name` being the **Name** of the physics interface (for example, `dl`).

COORDINATE SYSTEM SELECTION

Select a coordinate system from the **Coordinate system** list to specify the coordinate system in which the contributing velocity field is given. The default is the **Global coordinate system**. Note that the coordinate system used to specify the components of the contributing velocity field can be selected independently of the coordinate system of the parent feature.

CONTRIBUTING VELOCITY

The default contributing velocity field $\mathbf{u}_{\text{ctrb}}$ is **User defined**, which lets you enter the components of the contributing velocity field explicitly. If a matching velocity field is announced by another feature, it will be available in the selection list.

ADVANCED

Select the **Frame** in which the contributing velocity field is specified. The default is the **Reference configuration**, which means that the velocity field follows the material under, for example, a rotation of the domain. If instead your contributing velocity field follows a fixed direction in space, select the **Deformed configuration**. This section is only displayed if **Advanced Physics Options** is activated and the spatial and material frame of the component differ, such as in the presence of a **Moving Mesh** or **Solid Mechanics** interface.

LOCATION IN USER INTERFACE

Context Menus

If the selected *porous medium feature* is Porous Medium, Unsaturated Porous Medium, or Dual Porosity Medium:

Darcy's Law > *porous medium feature* > **Contributing Velocity**
Richards' Equation > *porous medium feature* > **Contributing Velocity**

Ribbon

Physics tab with **Porous Medium**, **Unsaturated Porous Medium**, or **Dual Porosity Medium** selected:

Attributes > **Contributing Velocity**

Initial Values

The **Initial Values** node adds an initial value for the pressure that can serve as an initial condition for a transient simulation or as an initial guess for a nonlinear solver.

If you have the Subsurface Flow Module licensed, you can specify the pressure either directly or as an expression for the pressure head, H_p, or the hydraulic head, H; the hydraulic head and the pressure head relate to the pressure p as

$$H_p = \frac{p}{\rho g}; \quad H = H_p + D$$

where ρ is the fluid density (SI unit: kg/m^3); g denotes the acceleration of gravity (SI unit: m/s^2); and D is the elevation (SI unit: m).

INITIAL VALUES

Enter a value or expression for the initial value of the **Pressure** p (SI unit: Pa). The default value is 0 Pa.

In case the Subsurface Flow Module is available, click the **Pressure head** button to enter a value or expression for H_p (SI unit: m). The default is 0 m. Click the **Hydraulic head** button to enter a value or expression for H (SI unit: m). The default is 0 m.

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Initial Values**

Richards' Equation > **Initial Values**

Ribbon

Physics tab with *interface* as **Darcy's Law** or **Richards' Equation** selected:

Domains > *interface* > **Initial Values**

Gravity

The **Gravity** node is automatically added when **Include gravity** is selected at interface level in the **Darcy's Law** settings and it is active in all domains in which the Darcy's Law interface is applied.

COORDINATE SYSTEM SELECTION

The **Global coordinate system** is selected by default. The **Coordinate system** list contains any additional coordinate systems that the model includes. It can be used when prescribing the direction of the gravitational forces.

GRAVITY

Specify either the acceleration vector or — in case you have a Subsurface Flow Module license — the elevation.

When **Acceleration** is selected from the list, enter the components of the **Gravity vector g**. The default value is `g_const` which is the physical constant having the value 9.8066 m/s^2.

- For 3D and 2D axisymmetric models, the default value is `-g_const` in the z direction.
- For 2D models, the default value is `-g_const` in the y direction.

When **Elevation** is selected from the list, specify the **Elevation** D (SI unit: m). The **Acceleration of gravity** is taken **From physics interface** by default but could be overridden when **User defined** is selected.

When the checkbox **Include gravity** is not selected in the Darcy's Law interface Settings, the elevation D is set equal to zero.

Select the checkbox **Specify reference position** to define a reference position for the gravity calculation.

LOCATION IN USER INTERFACE

Context Menus
Darcy's Law > **Gravity**
Richards' Equation > **Gravity**

Cross Section

Use this node with 1D components to model domains with another cross-sectional area than the global one that is used in the interface **Physical Model** section. In 1D geometries, the pressure is assumed to be constant in the radial direction, and Darcy's Law accounts for that.

CROSS SECTION

Enter values for the **Cross-sectional area** A_c to set the cross section of the domain in the plane perpendicular to the 1D geometry.

LOCATION IN USER INTERFACE

Context Menus
Darcy's Law > **Cross Section**
Richards' Equation > **Cross Section**

Ribbon

Physics tab with *interface* as **Darcy's Law** or **Richards' Equation** selected:

Domains > *interface* > **Cross Section**

Thickness

Use this node with 2D and 1D axisymmetric components to model domains with another thickness than the overall thickness that is specified in the interface **Physical Model** section. In 2D geometries, the pressure is assumed to be constant in the out-of-plane direction (the z direction with default spatial coordinate names). In 1D axisymmetric geometries the thickness represents the z direction.

THICKNESS

Specify a value for the **Thickness** d_z of the domain in the out-of-plane direction. This value replaces the overall thickness in the domains that are selected in the **Domain Selection** section, and is used to multiply some terms into the heat equation.

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Thickness**

Richards' Equation > **Thickness**

Ribbon

Physics tab with *interface* as **Darcy's Law** or **Richards' Equation** selected:

Domains > *interface* > **Thickness**

Porous Electrode Coupling

Use the **Porous Electrode Coupling** node to define a mass source based on the volumetric current densities of one or multiple **Porous Electrode Reaction** nodes in an Electrochemistry interface.

The source (or sink) is proportional to the **Molar mass (kg/mol)** of the reacting species, the current densities and the stoichiometric coefficients according to Faraday's law as defined by summation over the Reaction Coefficient subnodes.

SPECIES

Based on the number of species required for the model, use the **Add** (+) and **Delete**) buttons under the table to add or remove **Species**. Then enter a value for the **Molar mass (kg/mol)** in the applicable rows for each species.

The setting in the table will determine the number of available fields for entering the stoichiometric coefficients of the Reaction Coefficient subnodes.

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Porous Electrode Coupling**

Richards' Equation > **Porous Electrode Coupling**

Ribbon

Physics tab with *interface* as **Darcy's Law** or **Richards' Equation** selected:

Domains > *interface* > **Porous Electrode Coupling**

Electrode Surface Coupling

Use the **Electrode Surface Coupling** node to define a combined wall and inflow/outflow boundary condition based on current densities of one or multiple Electrode Reaction nodes in an Electrochemistry interface.

The flow is proportional to the **Molar mass (kg/mol)** of the reacting species, the current densities and the stoichiometric coefficients according to Faraday's law as defined by summation over the Reaction Coefficient subnodes.

SPECIES

Based on the number of species required for the model, use the **Add** (+) and **Delete**) buttons under the table to add or remove **Species**. Then enter a value for the **Molar mass (kg/mol)** in the applicable rows for each species.

The setting in the table will determine the number of available field for entering the stoichiometric coefficients of the Reaction Coefficient subnodes.

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Electrode Surface Coupling**

Richards' Equation > **Electrode Surface Coupling**

Ribbon

Physics tab with *interface* as **Darcy's Law** or **Richards' Equation** selected:

Boundaries > *interface* > **Electrode Surface Coupling**

Pressure

Use the **Pressure** node to specify the pressure on a boundary. In many cases the distribution of pressure is known, giving a Dirichlet condition $p = p_0$ where p_0 is a known pressure given as a number, a distribution, or an expression involving time, t, for example.

PAIR SELECTION

If this node is selected from the **Pairs** menu, choose the pair to apply this condition to. A pair must be created first. See Identity, Contact, and Sector Symmetry Pairs in the *COMSOL Multiphysics Reference Manual* for more details.

PRESSURE

Enter a value or expression for the **Pressure** p_0 (SI unit: Pa). Enter a relative pressure value in p_0 (SI unit: Pa).

For the Subsurface Flow Module, the **Pressure** node provides the pressure P_0 as a condition on edges in 3D models. Then select the edges under **Edge Selection**.

CONSTRAINT SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog.

As an attribute to the Fracture boundary condition or as boundary condition to The Fracture Flow Interface (which are available in the Subsurface Flow Module and the Porous Media Flow Module), the pressure can also be specified on edges (in 3D) or points (in 2D) surrounding the fracture domain. In other cases, pressure constraints on edges or points are not implemented.

!	If the boundary condition is adjacent to an Unsaturated Dual Permeability Medium feature it constrains the pressures in the Macropores and Micropores to p_0.

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Pressure**

Richards' Equation > **Pressure**

Ribbon

Physics tab with *interface* as **Darcy's Law** or **Richards' Equation** selected:

Boundaries > *interface* > **Pressure**

Pairs > *interface* > **Pressure**

Mass Flux

Use the **Mass Flux** node to specify the mass flux into or out of the model domain through some of its boundaries. It is often possible to determine the mass flux from the pumping rate or from measurements. With this boundary condition, positive values correspond to flow into the model domain:

$$\mathbf{n} \cdot \rho \frac{\kappa}{\mu}(\nabla p + \rho g \nabla D) = N_0$$

where N_0 is a value or expression for the specified inward (or outward) Darcy flux. D is the elevation head which is set to zero for other than Subsurface Flow Module applications.

MASS FLUX

Enter a value or expression for the **Inward mass flux** N_0. A positive value of N_0 represents an inward mass flux whereas a negative value represents an outward mass flux. The units are based on the geometric entity: **Boundaries**: (SI unit: kg/(m^2·s)).

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Mass Flux**

Richards' Equation > **Mass Flux**

Ribbon

Physics tab with *interface* as **Darcy's Law** or **Richards' Equation** selected:

Boundaries > *interface* > **Mass Flux**

Line Mass Source

The **Line Mass Source** node adds mass flow originating from a tube of infinitely small radius.

SELECTION

The **Line Mass Source** feature is available for all dimensions, but the applicable selection differs between the dimensions.

MODEL DIMENSION	APPLICABLE GEOMETRICAL ENTITY
2D	Points
2D Axisymmetry	Points not on the symmetry axis
3D	Edges

LINE MASS SOURCE

Enter a value or expression for the source strength, N_0 (SI unit: kg/(m·s)). A positive value results in mass injection from the line into the computational domain, and a negative value means that the mass is removed from the computational domain.

Line sources located on a boundary affect the adjacent computational domains. This effect makes the physical strength of a line source located in a symmetry plane twice the given strength.

Fracture Flow

The equivalent feature available for fracture flow is the **Mass Source** attribute of the Fracture boundary condition and the **Mass Source** point feature of the Fracture Flow Interface, both available in 3D only.

LOCATION IN USER INTERFACE

According to the model dimension as mentioned in Selection, this feature is available for the *geometrical entities* **Edges** or **Points**.

Context Menus

Darcy's Law > *geometrical entity* > **Line Mass Source**

Richards' Equation > *geometrical entity* > **Line Mass Source**

Ribbon

Physics tab with **Darcy's Law** or **Richards' Equation** selected:

geometrical entity > **Line Mass Source**

Point Mass Source

The **Point Mass Source** node models mass flow originating from an infinitely small sphere centered around a point. It is available for points in 3D geometries.

POINT MASS SOURCE

Enter a value or expression for the source strength, N_0 (SI unit: kg/(s)). A positive value results in mass injection from the point into the computational domain, and a negative value means that the mass is removed from the computational domain.

Point sources located on a boundary or on an edge affect the adjacent computational domains. This has the effect, for example, that the physical strength of a point source located in a symmetry plane is twice the given strength.

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Points** > **Point Mass Source**

Richards' Equation > **Points** > **Point Mass Source**

Ribbon

Physics tab with **Darcy's Law** or **Richards' Equation** selected:

Points > **Point Mass Source**

Inlet

The **Inlet** node adds a boundary condition for the inflow (or outflow) perpendicular (normal) to the boundary. It has three options that can be used to specify inlet condition on a boundary, as follows:

VELOCITY

Enter a value or expression for the **Normal inflow velocity** U_0 (SI unit: m/s). A positive value of U_0 represents an inflow velocity. A negative value represents an outflow velocity. The inlet velocity boundary condition is implemented as;

$$\mathbf{n} \cdot \rho \frac{\kappa}{\mu}(\nabla p + \rho g \nabla D) = \rho U_0$$

where U_0 is a value or expression for the specified inward (or outward) Darcy velocity. A positive value of the velocity U_0 corresponds to flow into the model domain whereas

a negative value represents an outflow. D is the elevation head which is set to zero for other than Subsurface Flow Module applications.

PRESSURE

Use the **Pressure** option to specify the inlet pressure on a boundary. In many cases the distribution of pressure is known, giving a Dirichlet condition $p = p_0$ where p_0 is a known pressure given as a number, a distribution, or an expression involving time, t, for example. Enter a value or expression for the **Pressure** p_0 (SI unit: Pa).

MASS FLOW

If you select **Mass flow** as the inlet condition, specify the total **Mass flow rate** M_0 (SI unit: kg/s), or the **Pointwise mass flux** N_0 (SI unit: kg/(m^2·s)).

With **Mass flow rate** boundary condition, positive values correspond to flow into the model domain:

$$-\int_{\partial\Omega} \rho(\mathbf{u}\cdot\mathbf{n})\mathrm{d}S = M_0$$

where M_0 is a value or expression for the specified inward (or outward) Darcy flux.

Pointwise mass flux boundary condition, positive values correspond to flow into the model domain:

$$\mathbf{n}\cdot\rho\frac{\kappa}{\mu}(\nabla p + \rho g\nabla D) = N_0$$

where N_0 is a value or expression for the specified inward (or outward) Darcy flux.

CONSTRAINT SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog.

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Inlet**

Richards' Equation > **Inlet**

Ribbon

Physics tab with *interface* as **Darcy's Law** or **Richards' Equation** selected:

Boundaries > *interface* > **Inlet**

Symmetry

The **Symmetry** node describes a symmetry boundary. The following condition implements the symmetry condition on an axis or a flow divide:

$$\mathbf{n} \cdot \frac{\kappa}{\mu} \nabla p = 0$$

$$\mathbf{n} \cdot \frac{\kappa}{\mu} (\nabla p + \rho g \nabla D) = 0$$

For axisymmetric components, COMSOL Multiphysics takes the axial symmetry boundaries (at $r = 0$) into account and automatically adds an **Axial Symmetry** node that is valid on the axial symmetry boundaries only.

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Symmetry**

Richards' Equation > **Symmetry**

Ribbon

Physics tab with *interface* as **Darcy's Law** or **Richards' Equation** selected:

Boundaries > *interface* > **Symmetry**

No Flow

The **No Flow** node is the default boundary condition stating that there is no flow across impermeable boundaries. The mathematical formulation is:

$$\mathbf{n} \cdot \rho \frac{\kappa}{\mu} (\nabla p + \rho g \nabla D) = 0$$

where $\mathbf{n}$ is the vector normal to the boundary. D is the elevation head which is set to zero for any other than Subsurface Flow Module applications.

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **No Flow**

Richards' Equation > **No Flow**

Ribbon

Physics tab with *interface* as **Darcy's Law** or **Richards' Equation** selected:

Boundaries > *interface* > **No Flow**

Flux Discontinuity

Use the **Flux Discontinuity** node to specify a mass flux discontinuity through an interior boundary. The condition is represented by the following equation:

$$-\mathbf{n} \cdot (\rho \mathbf{u}_1 - \rho \mathbf{u}_2) = N_0$$

In this equation, $\mathbf{n}$ is the vector normal (perpendicular) to the interior boundary, ρ is the fluid density, $\mathbf{u}_1$ and $\mathbf{u}_2$ are the Darcy velocities in the adjacent domains (as defined in Equation 6-11) and N_0 is a specified value or expression for the flux discontinuity.

$$\mathbf{u} = -\frac{\kappa}{\mu}\nabla p \tag{6-11}$$

For this boundary condition, a positive value of N_0 corresponds to a flow discontinuity in the opposite direction to the normal vector of the interior boundary.

MASS FLUX

Enter a value or expression for the **Inward mass flux** N_0 (SI unit: $\mathrm{kg}/(\mathrm{m}^2 \cdot \mathrm{s})$). A positive value of N_0 represents a mass flux discontinuity in the opposite direction to the normal vector of the interior boundary.

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Interior Surfaces** > **Flux Discontinuity**

Richards' Equation > **Interior Surfaces** > **Flux Discontinuity**

Ribbon

Physics tab with **Darcy's Law** or **Richards' Equation** selected:

Boundaries > **Interior Surfaces** > **Flux Discontinuity**

Pairs > **Flux Discontinuity**

Outlet

The **Outlet** node adds a boundary condition for the outflow (or inflow) perpendicular (normal) to the boundary. It has different options that can be used to specify inlet condition on a boundary, as follows:

VELOCITY

Enter a value or expression for the **Normal outflow velocity** U_0 (SI unit: m/s). A positive value of U_0 represents an outflow velocity whereas a negative value represents an inflow velocity.

$$-\mathbf{n} \cdot \rho \frac{\kappa}{\mu} \nabla p = \rho U_0$$

where U_0 is a specified value or expression for the outward (or inward) Darcy velocity.

PRESSURE

Similar to the inlet **Pressure** option, the outlet pressure on a boundary can be specified. Enter a value or expression for the **Pressure** p_0 (SI unit: Pa).

DISCHARGE

Enter a value or expression for the discharge Q_D to specify the volumetric flow rate through the boundary. The mass flux $\rho\mathbf{u}$ is related to the discharge as follows:

$$\int_{\partial\Omega} \rho \mathbf{u} \cdot \mathbf{ds} = \rho Q_D . \tag{6-12}$$

The mean normal outflow velocity at the boundary can then be calculated as $U_\mathrm{out} = Q_\mathrm{D}/A$, where A is the cross sectional area of the boundary.

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Outlet**

Richards' Equation > **Outlet**

Ribbon

Physics tab with *interface* as **Darcy's Law** or **Richards' Equation** selected:

Boundaries > *interface* > **Outlet**

Precipitation

The **Precipitation** node adds a boundary condition for the inflow (of rain) perpendicular (normal) to the boundary.

Enter a value or expression for the **Precipitation rate** which then contributes to the mass flux at the selected boundaries.

Select the **Slope correction** checkbox to apply a correction that depends on the normal to the boundary and the vertical axis. This is needed when the boundary is inclined.

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Hydraulics** > **Precipitation**

Richards' Equation > **Hydraulics** > **Precipitation**

Ribbon

Physics tab with **Darcy's Law** or **Richards' Equation** selected:

Boundaries > **Hydraulics** > **Precipitation**

Interior Wall

The **Interior Wall** boundary condition can only be applied on interior boundaries. It is similar to the **No Flux** boundary available on exterior boundaries except that it applies on both sides of an interior boundary. It allows discontinuities of velocity and pressure across the boundary. The **Interior Wall** boundary condition can be used to avoid meshing thin structures by applying no-flux condition on interior curves and surfaces instead.

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Interior Surfaces** > **Interior Wall**

Richards' Equation > **Interior Surfaces** > **Interior Wall**

Ribbon

Physics tab with **Darcy's Law** or **Richards' Equation** selected:

Boundaries > **Interior Surfaces** > **Interior Wall**

Thin Barrier

The **Thin Barrier** boundary condition models interior permeable walls, membranes, geotextiles, or perforated plates as thin permeable barriers. The **Thin Barrier** boundary condition can only be applied on interior boundaries.

WALL

Enter a value or expression for the **Thickness** d_b (SI unit: m, the default is 0.1 m) and for the **Permeability** $\tilde{\kappa}_b$ (SI unit: m^2). The default **Permeability** $\tilde{\kappa}_b$ uses the value **From material**. For **User defined** select **Isotropic** to define a scalar value or **Diagonal**, **Symmetric**, or **Full** to define a tensor value and enter another value or expression in the field or matrix.

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Interior Surfaces** > **Thin Barrier**

Richards' Equation > **Interior Surfaces** > **Thin Barrier**

Ribbon

Physics tab with **Darcy's Law** or **Richards' Equation** selected:

Boundaries > **Interior Surfaces** > **Thin Barrier**

Pressure Head

Use the **Pressure Head** node to specify the pressure head (instead of the pressure) on a boundary. It adds this boundary condition for the pressure head $H_p = H_{p0}$, where H_{p0} is a known pressure head given as a number, a distribution, or an expression involving time, t, for example. The dimension of the pressure head is length (SI unit: m).

PRESSURE HEAD

Enter a value or expression for the **Pressure head** H_{p0} (SI unit: m). The default is 0 m.

CONSTRAINT SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog.

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Hydraulics** > **Pressure Head**
Richards' Equation > **Hydraulics** > **Pressure Head**

Ribbon

Physics tab with **Darcy's Law** or **Richards' Equation** selected:

Boundaries > **Hydraulics** > **Pressure Head**
Pairs > **Pressure Head**

Hydraulic Head

Use the **Hydraulic Head** node to specify the hydraulic head (instead of the pressure) on a boundary. This adds the Dirichlet condition for the hydraulic head $H = H_0$ where H_0 is a known hydraulic head given as a number, a distribution, or an expression involving time, t, for example.

HYDRAULIC HEAD

Enter a value or expression for the **Hydraulic head** H_0 (SI unit: m). The default is 0 m.

CONSTRAINT SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog.

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Hydraulics** > **Hydraulic Head**
Richards' Equation > **Hydraulics** > **Hydraulic Head**

Ribbon

Physics tab with **Darcy's Law** or **Richards' Equation** selected:

Boundaries > **Hydraulics** > **Hydraulic Head**
Pairs > **Hydraulic Head**

Atmosphere/Gauge

The **Atmosphere/Gauge** node specifies an atmospheric pressure or gauges the pressure to the atmospheric value. This means that the total hydraulic potential reduces to the

gravitational pressure at the free surface. At a free surface, such as a spring or a seepage face, the pressure is atmospheric. If the pressures in the model is gauged to the atmospheric value ($p = 0$), the total hydraulic potential reduces to the gravitational potential at the free surface — for example, the height of the free surface multiplied by the fluid weight, or $\rho_f g D$. This boundary condition sets the pressure at the boundary to zero and $p = 0$.

CONSTRAINT SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog.

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Hydraulics** > **Atmosphere/Gauge**

Richards' Equation > **Hydraulics** > **Atmosphere/Gauge**

Ribbon

Physics tab with **Darcy's Law** or **Richards' Equation** selected:

Boundaries > **Hydraulics** > **Atmosphere/Gauge**

Pervious Layer

The **Pervious Layer** node provides a boundary condition that describes a mass flux through a semi-pervious layer connected to an external fluid source at different pressure, pressure head, or hydraulic head. The model domain might connect to a larger body of water through the semi-pervious layer. This condition is represented with the following boundary condition:

$$\mathbf{n} \cdot \rho \frac{\kappa}{\mu}(\nabla p + \rho g \nabla D) = \rho R_b \left[\frac{(p_b - p)}{\rho g} + (D_b - D) \right] \tag{6-13}$$

In this equation, p_b (SI unit: Pa) and D_b (SI unit: m) are the pressure and the elevation of the distant fluid source, respectively, and R_b (SI unit: 1/s) is the conductance of materials between the source and the model domain (conductance to flow in the semi-pervious layer adjacent to the boundary). Typically $R_b = K'/B'$, where K' is the hydraulic conductivity (SI unit: m/s) of the layer and B' (SI unit: m) is its thickness. Using logical relationships, it is possible to activate these expressions at different times or under various flow conditions.

When the pressure head H_p is specified instead of the pressure, the boundary condition is the following:

$$\mathbf{n} \cdot \rho K \nabla (H_p + D) = \rho R_\mathrm{b}[(H_{p\mathrm{b}} - H_p) + (D_\mathrm{b} - D)] \tag{6-14}$$

H_{pb} is the pressure head (SI unit: m) at the edge of the layer.

When the hydraulic head H is specified instead of the pressure head, the boundary condition becomes:

$$\mathbf{n} \cdot \rho K \nabla H = \rho R_\mathrm{b}[H_\mathrm{b} - H] \tag{6-15}$$

H_b is the hydraulic head (SI unit: m) at the edge of the layer.

K in Equation 6-14 and Equation 6-15 is the hydraulic conductivity.

At a free surface, such as a water table or seepage face, the pressure is atmospheric (here taken to be zero), so the total hydraulic potential equals gravitational potential, which is defined on D.

	Gravity effects are not active by default. Select the checkbox **Include gravity** to activate the acceleration of gravity. Setting the elevation D to zero also turns off gravity effects.

PERVIOUS LAYER

Specify the material properties whether to specify an external pressure, pressure head, or hydraulic head.

Select an **External variable to specify** — **Pressure and elevation** to specify the external pressure, **Pressure head and elevation** to specify the external pressure head, or **Hydraulic head**. For all selections, enter a value for the **Conductance** R_b (SI unit: 1/s).

- For **Pressure and elevation** enter an **External pressure** p_b (SI unit: Pa) and **External elevation** $D_\mathbf{b}$ (SI unit: m).
- For **Pressure head and elevation** enter an **External pressure head** $H_{p\mathrm{b}}$ (SI unit: m), $H_{p\mathrm{b}}$ (SI unit: m) and **External elevation** D_b (SI unit: m).
- For **Hydraulic head** enter the **Hydraulic head** H_b (SI unit: m).

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Hydraulics** > **Pervious Layer**

Richards' Equation > **Hydraulics** > **Pervious Layer**

Ribbon

Physics tab with **Darcy's Law** or **Richards' Equation** selected:

Boundaries > **Hydraulics** > **Pervious Layer**

Well

The **Well** feature is intended to model injection or production wells and is available with the Subsurface Flow Module.

WELL

Enter a value or expression for the **Well diameter** d_w (SI unit: m, the default is 0.1 m). Select the **Well type** from the list: **Production** or **Injection**.

Specify either the **Pressure** (SI unit: Pa), **Pressure head** (SI unit: m), **Hydraulic head** (SI unit: m), or the **Mass flow**. If you select **Mass flow**, specify the total **Mass flow rate** (SI unit: kg/s), the **Mass flow rate per unit length** (SI unit: kg/(m·s)) or the **Mass flux** (SI unit: kg/(m^2·s)).

LOCATION IN USER INTERFACE

According to the model dimension this feature is available for the *geometrical entities* **Edges** (3D) or **Points** (2D).

Context Menus

Darcy's Law > *geometrical entity* > **Well**
Richards' Equation > *geometrical entity* > **Well**

Ribbon

Physics tab with **Darcy's Law** or **Richards' Equation** selected:

geometrical entity > **Well**

Fracture

Use the **Fracture** node to model flow along a boundaries representing fractures within a porous medium. By default, it adds the tangential form of the continuity equation and of Darcy's Law.

$$d_f \frac{\partial}{\partial t}(\varepsilon_p \rho) + \nabla_T \cdot (d_f \rho \mathbf{u}) = d_f Q_m \tag{6-16}$$

$$\mathbf{u} = -\frac{\kappa}{\mu}\nabla_T p \tag{6-17}$$

The **Fracture** feature has two default subfeatures — the Fluid (Fracture) subfeature where the fluid density ρ (SI unit: kg/m^3) and dynamic viscosity μ (SI unit: Pa·s) are defined and the Fracture Material subfeature where the permeability κ (SI unit: m^2) and porosity ε_p (dimensionless) are specified.

COORDINATE SYSTEM SELECTION

Select a coordinate system from the **Coordinate system** list for the interpretation of directions in anisotropic material properties. The default is the **Global coordinate system**, and the list contains any additional orthonormal coordinate system (except boundary coordinate systems) added under the **Definitions** node.

The subnodes inherit these coordinate system settings. In particular, the **Permeability** or **Hydraulic conductivity** (in the Fracture Material subnode) should be set according to the coordinate system selected in this section.

APERTURE

Enter a value for the **Fracture thickness** d_f.

FLOW MODEL

Define if the flow follows a linear or nonlinear pressure-velocity relationship.

- **Darcian flow** (default) defines a linear relationship using Equation 6-16 and Equation 6-17.
- **Non-Darcian flow** defines a nonlinear relationship using Equation 6-16 and the pressure-velocity relationship

$$\nabla_T p = -\frac{\mu}{\kappa}\mathbf{u} - \beta\rho|\mathbf{u}|\mathbf{u}$$

  where the nonlinear parameter β (SI unit: $1/m$) is further specified in the Fracture Material subfeature.

STORAGE MODEL

Equation 6-16 can also be formulated with respect to a storage term.

$$\rho S\frac{\partial p}{\partial t} + \nabla \cdot \rho\left[-\frac{\kappa}{\mu}(\nabla p)\right] = Q_m$$

The storage coefficient S can be interpreted as the weighted compressibility of the porous material and the fluid. Define the time dependent storage term by selecting one of the following options from the list:

- **From density and porosity** (default), uses the formulation of Equation 6-16
- **Linearized storage**, where the following linear equation is used to define the storage:

$$S = \varepsilon_p \chi_f + (1 - \varepsilon_p)\chi_p$$

- **User defined** to directly specify the storage coefficient S

- About Darcian and Non-Darcian Flow in the *Porous Media Flow Module User's Guide*
- Storage Models in the *Subsurface Flow Module User's Guide*

FRACTURE MODEL

Choose between two options to model fractures that have different characteristics.

- **Highly conductive fracture** represents a fracture filled with a highly permeable material.
- **Thin conducting barrier** represents a fracture that is filled with a low permeable material and therefore acts as a barrier for the flow which adds a jump in the pressure across the boundary:

$$-\mathbf{n}_{u,d} \cdot (\rho \mathbf{u})_{u,d} = \rho \frac{(p_{d,u} - p_{u,d})}{d_b} \frac{\kappa_b}{\mu}$$

  The barrier thickness d_b and permeability κ_b are defined in the Fracture Material subnode.

  In addition, either on the upside, downside, or on both sides a highly conductive fracture material is present and Equation 6-16 and Equation 6-17 are solved for the highly conductive side. Further specifications are done in the Fracture Material subnode.

Note that the option to specify the **Fracture Model** is only available for the Fracture feature within the Darcy's Law interface.

For the Fracture boundary node several subnodes are available from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu. As they are

almost identical to the boundary conditions of the Fracture Flow interface, see Domain, Boundary, Edge, Point, and Pair Nodes for the Fracture Flow Interface in the *Subsurface Flow User's Guide* for further description. Note that **Precipitation** is only available for the Fracture Flow interface.

	This feature requires a specific license. For a detailed overview of the functionality available in each product, visit https://www.comsol.com/products/specifications/.

	Flow in a Fractured Reservoir: Application Library path **Subsurface_Flow_Module/Fluid_Flow/fractured_reservoir_flow**

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Fracture**

Richards' Equation > **Fracture**

Fracture Flow > **Fracture**

Ribbon

Physics tab with *interface* as **Darcy's Law** or **Richards' Equations** selected:

Boundaries > *interface* > **Fracture**

With **Fracture Flow** selected:

Boundaries > **Fracture**

Fluid (Fracture)

This node defines the material properties of the fluid of the Fracture parent node. The fluid can be specified as general gas or liquid or as an ideal gas.

MODEL INPUT

This section contains fields and values that are inputs for expressions defining material properties. If such user-defined property groups are added, the model inputs appear here.

FLUID PROPERTIES

The available options for the **Fluid type** are **Gas/Liquid** (default) or **Ideal gas**. The selection determines how the density and compressibility of the fluid are set. The latter is only required if a linearized storage model has been selected in the parent Fracture node. For all fluid types specify the dynamic viscosity μ (SI unit: Pa·s).

Gas/Liquid

This option specifies the **Density** and the **Compressibility** for a general gas or liquid.

Ideal Gas

For **Ideal gas** it uses the ideal gas law to describe the fluid. In this case, specify the thermodynamics properties. Select a **Gas constant type** — **Specific gas constant** R_s (the default) or **Mean molar mass** M_n (SI unit: J/(mol·K)). For **Mean molar mass** the universal gas constant $R = 8.314$ J/(mol·K) is used as the built-in physical constant. For both properties, the defaults use values **From material**. For **User defined** enter another value or expression.

If required by a **Storage Model**, the **Compressibility** of the ideal gas is calculated as $\chi_f = 1/p_A$ with the absolute pressure p_A (Pa).

If **Hydraulic conductivity** is selected as the **Permeability model** (see the Fracture Material section), dynamic viscosity is not available. The hydraulic conductivity is defined using a combination of fluid and fracture material properties and replaces the need of defining the dynamic viscosity.

LOCATION IN USER INTERFACE

A default **Fluid** node is automatically added to the Fracture node.

Context Menus

Darcy's Law > **Fracture** > **Fluid**

Richards' Equation > **Fracture** > **Fluid**

Fracture Flow > **Fracture** > **Fluid**

Fracture Material

This node defines the porosity and material properties of the solid matrix of the Fracture parent node.

MODEL INPUT

This section contains fields and values that are inputs for expressions defining material properties. If such user-defined property groups are added, the model inputs appear here.

BARRIER PROPERTIES

This section appears if the **Thin conducting barrier** option for the **Fracture model** is chosen in the parent Fracture feature.

Enter the values for the barrier thickness d_b and permeability κ_b.

Note that the **Thin Conductive barrier** option is only available for the Fracture feature within the Darcy's Law interface.

FRACTURE MATERIAL PROPERTIES

If the **Thin conducting barrier** option for the **Fracture model** is chosen in the parent Fracture feature you can specify the **Conductive layer position** here. Choose between **Both sides**, **Upside**, and **Downside**. A sketch above shows the position of conductive layers and barrier within the fracture.

The **Porosity** ε_p of the fracture material is taken **From material** by default. Select **User defined** to enter a value or expression for ε_p.

If required by a **Storage model** in the parent node, specify the **Effective compressibility** of the porous matrix. The default value is $\chi_p = 10^{-4}$ 1/Pa.

Select a **Permeability model** to specify the capacity of the fracture material to transmit flow. Which options are available depends on the **Flow model** setting in the parent node.

- Select **Permeability** (default) to define the permeability of the fracture material.
- Select **Hydraulic conductivity** or define a combination of fluid permeability and dynamic viscosity. For **Hydraulic conductivity** K (SI unit: m/s) select **Isotropic** to define a scalar value or **Diagonal** or **Symmetric** to define a tensor value. The default is $2.94 \cdot 10^{-4}$ m/s.
- Select **Cubic law** to define the permeability from the fracture thickness specified in the parent node and the roughness factor f_f.

If the Non-Darcian Flow Model is selected in the parent Fracture feature enter a value for the **Inertial resistance coefficient** β.

	• About Darcian and Non-Darcian Flow in the *Porous Media Flow Module User's Guide* • Permeability Models in the *Porous Media Flow Module User's Guide*

LOCATION IN USER INTERFACE

A default **Fracture Material** node is automatically added to the Fracture node.

Context Menus

Darcy's Law > **Fracture** > **Fracture Material**

Richards' Equation > **Fracture** > **Fracture Material**

Fracture Flow > **Fracture** > **Fracture Material**

The Brinkman Equations Interface

The **Brinkman Equations (br)** interface ( ), found under the **Porous Media and Subsurface Flow** branch ( ) when adding a physics interface, is used to compute fluid velocity and pressure fields of single-phase flow in porous media in the laminar flow regime. The physics interface extends Darcy's law to describe the dissipation of the kinetic energy by viscous shear, similar to the Navier–Stokes equations. Fluids with varying density can be included at Mach numbers below 0.3. Also the viscosity of a fluid can vary, for example, to describe non-Newtonian fluids. To simplify the equations, select the Stokes–Brinkman flow feature to reduce the dependence on inertial effects when the Reynolds number is significantly less than 1. The physics interface can be used for stationary and time-dependent analyses.

The main node is the Porous Medium feature, which adds the Brinkman equations and provides interfaces for defining the fluid material and the porous matrix.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Porous Medium**, **Wall** (the default boundary type, using **No slip** as the default boundary condition), and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and volume forces. You can also right-click **Brinkman Equations** to select physics features from the context menu.

The boundary conditions are essentially the same as for the Laminar Flow interface. Differences exist for the following boundary types: Outlet, Symmetry, Open Boundary, and Boundary Stress where the viscous part of the stress is divided by the porosity to appear as

$$\frac{1}{\varepsilon_p}\left\{\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)-\frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right\}$$

In the *COMSOL Multiphysics Reference Manual* see Table 2-4 for links to common sections such as **Discretization**, **Consistent Stabilization**, **Inconsistent Stabilization**, and **Advanced Settings**, all accessed by clicking the **Show** button ( ) and choosing the applicable option. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `br`.

PHYSICAL MODEL

This node specifies the properties of the Brinkman Equations interface, which describe the overall type of fluid flow model.

Compressibility

By default the physics interface uses the **Incompressible flow** formulation of the Brinkman equations to model constant density flow. Alternatively, from the **Compressibility** list select **Weakly compressible flow**, which should be used when the pressure dependency of the density can be neglected, or **Compressible flow (Ma<0.3)** to solve for the full compressible flow of which, however, the Mach number must be below 0.3.

Swirl Flow

For 2D axisymmetric models, select the **Swirl flow** checkbox to include the swirl velocity component, that is the velocity component u_φ in the azimuthal direction. While u_φ can be nonzero, there can be no gradients in the φ direction.

Note that this feature is only available for specific modules. See https://www.comsol.com/products/specifications/ for a detailed overview.

Neglect Inertial Term (Stokes–Brinkman Flow)

The **Neglect inertial term (Stokes–Brinkman)** checkbox is selected by default to model flow at low Reynolds numbers for which the inertial term can be neglected. This results in the linear Stokes–Brinkman equations.

Include Gravity

Gravity is not included by default. Select the **Include gravity** checkbox to activate the acceleration of gravity. This automatically adds a global **Gravity** feature node to the interface model tree, and the buoyancy force is included in the equations.

Also, when the **Include gravity** checkbox is selected, the **Use reduced pressure** option changes the pressure formulation from using the total pressure (default) to using the reduced pressure. This option is suitable for configurations where the density changes

are very small; otherwise, the default formulation can be used. For more information, see Gravity.

Porous Treatment of No Slip Condition

Choose how the **No Slip** condition on **Wall** boundaries and **Interior Wall** boundaries adjacent to **Porous Medium** should be treated. The options are **Standard no slip formulation** and **Porous slip** (the default). The latter option provides a unified treatment when the porous matrix is fully resolved as well as when it is under resolved ensuring a smooth transition between regions with different resolutions; see No Slip under Wall in The Laminar Flow and Creeping Flow Interfaces section.

Reference Pressure Level

Enter a **Reference pressure level** p_{ref} (SI unit: Pa). The default value is `1[atm]`.

Reference Temperature Level

Enter a **Reference temperature level** T_{ref} (SI unit: K). The default value is `293.15[K]`.

Reference Position

If **Include gravity** is selected, a **Reference position** r_{ref} (SI unit: m) can be specified which is then used for the calculation of the hydrostatic pressure.

TURBULENCE

Turbulent flow can be simulated by changing the **Turbulence model type** to **RANS-EVM** (Reynolds-Averaged Navier–Stokes, eddy-viscosity model). If **RANS-EVM** is activated, you can set the **Turbulence model** either to one of the algebraic turbulence models, **Algebraic yPlus** (the default) or **L-VEL**, or to one of the following two-equation turbulence models: k-ε, Low Reynolds Number k-ε. The **Wall treatment** is set to **Automatic** (default) or **Low Re** while **Wall functions** is the only option for k-ε.

For more information about turbulence modeling, see Theory for the Turbulent Flow Interfaces in the *CFD Module User's Guide*.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface — the **Velocity field** $\mathbf{u}$ (SI unit: m/s) and its components, and the **Pressure** p (SI unit: Pa).

ADVANCED SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog. Normally these settings do not need to be changed.

The **Use pseudo time stepping for stationary equation form** option adds pseudo time derivatives to the equation when the **Stationary equation** form is used in order to speed up convergence. When selected, a **CFL number expression** should also be defined. For the default **Automatic** option, the local CFL number (from the Courant–Friedrichs–Lewy condition) is determined by a PID regulator.

- Domain, Boundary, Point, and Pair Nodes for the Brinkman Equations Interface
- Theory for the Brinkman Equations Interface
- Pseudo Time Stepping for Laminar Flow Models and Pseudo Time Stepping in the *COMSOL Multiphysics Reference Manual*
- Numerical Stability — Stabilization Techniques for Fluid Flow
- Nitsche Constraints

Domain, Boundary, Point, and Pair Nodes for the Brinkman Equations Interface

The Brinkman Equations Interface has the following domain, boundary, point, and pair nodes, listed in alphabetical order, available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

These nodes are described in this section:

- Porous Medium
- Initial Values
- Mass Source
- Volume Force
- Fluid Properties

The following nodes (listed in alphabetical order) are described for the Laminar Flow interface :

- Flow Continuity
- Inlet
- Line Mass Source
- Boundary Stress
- Outlet
- Open Boundary
- Periodic Flow Condition
- Point Mass Source
- Pressure Point Constraint
- Symmetry
- Wall

!	In the *COMSOL Multiphysics Reference Manual* see Table 2-4 for links to common sections and Table 2-5 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Porous Medium

The **Porous Medium** node adds the Brinkman equations: Equation 4-34 and Equation 4-35 (excluding any mass sources). It has two default subfeatures — the Fluid subfeature where the fluid density ρ(SI unit: kg/m^3) and dynamic viscosity μ (SI unit: Pa·s) are defined and the Porous Matrix subfeature where the permeability κ (SI unit: m^2) and porosity ε_p (dimensionless) are specified.

COORDINATE SYSTEM SELECTION

Select a coordinate system from the **Coordinate system** list for the interpretation of directions in anisotropic material properties. The default is the **Global coordinate system**, and the list contains any additional orthonormal coordinate system (except boundary coordinate systems) added under the Definitions node.

The subnodes inherit these coordinate system settings. In particular, the **Permeability** (in the **Porous Matrix** subnode) should be set according to the coordinate system selected in this section.

FLOW MODEL

Define if the flow follows a linear or nonlinear pressure-velocity relationship.

- **Darcian flow** (default) defines a linear relationship characteristic for low Reynolds number laminar flows.
- **Non-Darcian flow** defines a nonlinear relationship due to inertial or turbulence effects.

POROUS MEDIUM TURBULENCE MODEL

If in the parent feature node a turbulence model other than **Algebraic yPlus** or **L-VEL** is selected, define a model which complements the basic turbulence model and accounts for the influence of the porous matrix on turbulent flow in porous media.

- For **Default** and **Nakayama-Kuwahara** specify the **Coefficient of subgrid turbulence generation by porous matrix** C_{stpm} which by default is set to 0.212.
- For **Pedras-de Lemos**, specify the **Choice of the Pedras-de Lemos model coefficient**. When **User defined** is chosen, specify the **Coefficient of subgrid turbulence generation by porous matrix** C_{stpm} with default value 0.212. Choosing **Original** results in $C_{stpm} = 0.28 \cdot \sqrt{\varepsilon_p}$, while choosing **Recalibrated** results in $C_{stpm} = 0.18$.
- If **Turbulence model type** is **RANS-RSM**, specify the **Production of Reynolds stresses by porous matrix**. The default is **Isotropic** and the other option is **Streamwise**.

DISTANCE EQUATION

This section is available for the turbulence models **Algebraic yPlus** or **L-VEL**. Select how the **Reference length scale** l_{ref} (SI unit: m) is defined — **Automatic** (default) or **Manual**:

- For Automatic the wall distance is automatically evaluated to one tenth of the shortest side of the geometry bounding box. This is usually quite accurate but it can sometimes give a too high value if the geometry consists of several slim entities. In such cases, define the reference length scale manually.
- For Manual it defines a different value or expression for the length scale. The default is 1 m.

l_{ref} controls the result of the distance equation. Objects that are much smaller than l_{ref} are effectively be diminished while the distance to objects much larger than l_{ref} are accurately represented.

LOCATION IN USER INTERFACE

Context Menus

Brinkman Equations > **Porous Medium**

Ribbon

Physics tab with **Brinkman Equations** selected:

Domains > **Porous Medium**

Fluid

This node defines the material properties of the fluid of the Porous Medium parent node.

MODEL INPUT

This section contains fields and values that are inputs for expressions defining material properties. If such user-defined property groups are added, the model inputs appear here.

FLUID PROPERTIES

Specify the **Density** ρ and the **Dynamic viscosity** μ (SI unit: Pa·s) of the fluid. The defaults use values **From material**, for **User defined** enter a value or expression.

The dynamic viscosity describes the relationship between the shear stresses and the shear rate in a fluid. Intuitively, water and air have a low viscosity, and substances often described as thick, such as oil, have a higher viscosity.

If the Polymer Flow Module license is available and for Darcian flow, also non-Newtonian models are available and the **Constitutive Relation** can be switched between **Specify dynamic viscosity** (default) or **Inelastic non-Newtonian**.

Constitutive Relation

Use the default option to either get the dynamic viscosity from a material, or to add a user defined expression. The default option lets you either use the dynamic viscosity from a material or define it with a custom expression. The **Inelastic non-Newtonian** option provides several models and defines the **Apparent shear rate**.

Inelastic Non-Newtonian

The following inelastic non-Newtonian Models are available for the **Fluid** feature under the **Porous Medium** feature:

- Power Law

- Carreau
- Carreau-Yasuda
- Cross
- Cross-Williamson
- Sisko

The setup of these models in porous media is similar to their definition under the Fluid Properties feature.

Apparent Shear Rate

To define the apparent shear rate $\dot{\gamma}_{\text{app}}$, either enter a user-defined expression for the correction factor (α) or choose the **Capillary bundle approach** from the list and provide a value for the Tortuosity factor (C).

	• Read more about the theory of Non-Newtonian Fluids in Porous Media in the *Polymer Flow Module User's Guide*

LOCATION IN USER INTERFACE

A default **Fluid** node is automatically added to the Porous Medium node.

Context Menus

Brinkman Equations > **Porous Medium** > **Fluid**

Porous Matrix

This node defines the porosity and material properties of the solid matrix of the Porous Medium parent node.

MODEL INPUT

This section contains fields and values that are inputs for expressions defining material properties. If such user-defined property groups are added, the model inputs appear here.

MATRIX PROPERTIES

The **Porosity** ε_p (a dimensionless number between 0 and 1) uses by default the value **From material**. For **User defined** the default value is 1.

Select a **Permeability model** to specify the capacity of the porous material to transmit flow. Depending on the **Flow model** selection in the parent **Porous Medium** feature node you can choose between the following options:

- **Permeability** (the default) to directly enter the permeability of the porous matrix or **Kozeny-Carman** to define the permeability from the porosity and mean **Particle diameter** for **Darcian** flow or
- **Forchheimer** or **Ergun** for **Non-Darcian** flow.

Note that some of these options are only available for certain modules. For a detailed overview of the functionality available in each product, visit https://www.comsol.com/products/specifications/.

The default **Permeability** κ (SI unit: m^2) uses the value **From material**, as defined by the **Porous material** list. For **User defined** select **Isotropic** to define a scalar value or **Diagonal** or **Symmetric** to define a tensor value.

For **Kozeny-Carman**, enter the mean **Particle diameter** d_p (SI unit: m), the default value is 0.5 mm.

In case a **Non-Darcian** flow model is chosen in the parent node, **Forchheimer** is the default selection for the **Permeability model**. For **Forchheimer**, the default **Permeability** κ (SI unit: m^2) uses the value **From material**. Furthermore, the dimensionless **Forchheimer parameter** c_F can be defined. The default value is 0.55.

If **Ergun** is selected, enter the mean **Particle diameter** d_p (default value: 0.5 mm). The permeability κ is then calculated using Equation 2-4 in the *Porous Media Flow Module User's Guide*.

- About Darcian and Non-Darcian Flow in the *Porous Media Flow Module User's Guide*
- Permeability Models in the *Porous Media Flow Module User's Guide*

LOCATION IN USER INTERFACE

A default **Porous Matrix** node is automatically added to the Porous Medium node.

Context Menus

Brinkman Equations > **Porous Medium** > **Porous Matrix**

Mass Source

The **Mass Source** node adds a mass source (or mass sink) Q_m to the right-hand side of the continuity equation: Equation 6-28. This term accounts for mass deposit and/or mass creation in porous domains. The physics interface assumes that the mass exchange occurs at zero velocity.

$$\frac{\partial}{\partial t}(\varepsilon_p \rho) + \nabla \cdot (\rho \mathbf{u}) = Q_m \tag{6-18}$$

DOMAIN SELECTION

Only Porous Matrix domains are available.

MASS SOURCE

Enter a value or expression for the **Source term** Q_{br} (SI unit: kg/(m^3·s)). The default is 0 kg/(m^3·s).

LOCATION IN USER INTERFACE

Context Menus

Brinkman Equations > **Mass Source**

Ribbon

Physics tab with **Brinkman Equations** selected:

Domains > **Mass Source**

Volume Force

Use the **Volume Force** node to specify the force $\mathbf{F}$ on the right-hand side of Equation 6-29. It then acts on each fluid element in the specified domains.

$$\begin{aligned}&\frac{\rho}{\varepsilon_p}\left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\frac{\mathbf{u}}{\varepsilon_p}\right) = \\ &-\nabla p + \nabla \cdot \left[\frac{1}{\varepsilon_p}\left\{\mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I}\right\}\right] - \left(\kappa^{-1}\mu + \frac{Q_m}{\varepsilon_p^2}\right)\mathbf{u} + \mathbf{F}\end{aligned} \tag{6-19}$$

VOLUME FORCE

Enter the components of **Volume force** $\mathbf{F}$ (SI unit: N/m^3).

LOCATION IN USER INTERFACE

Context Menus
Brinkman Equations > **Volume Source**

Ribbon
Physics tab with **Brinkman Equations** selected:

Domains > **Volume Source**

Initial Values

The **Initial Values** node adds initial values for the velocity field and the pressure that can serve as an initial condition for a transient simulation or as an initial guess for a nonlinear solver.

INITIAL VALUES

Enter initial values or expressions for the **Velocity field** $\mathbf{u}$ (SI unit: m/s) and the **Pressure** p (SI unit: Pa). The default values are 0 m/s and 0 Pa, respectively.

LOCATION IN USER INTERFACE

Context Menus
Brinkman Equations > **Initial Values**

Ribbon
Physics tab with **Brinkman Equations** selected:

Domains > **Initial Values**

Fluid Properties

The **Fluid Properties** node adds the momentum and continuity equations to solve for free flow in nonporous domains. The node also provides an interface for defining the material properties of the fluid.

MODEL INPUTS

Fluid properties, such as density and viscosity, can be defined through user inputs, variables, or by selecting a material. For the latter option, additional inputs — for example, temperature or pressure — may be required to define these properties.

Temperature

By default, the single-phase flow interfaces are set to model isothermal flow. Hence, the **Temperature** is **User defined** and defaults to 293.15 K. If a Heat Transfer interface is included in the component, the temperature may alternatively be selected from this physics interface. All physics interfaces have their own tags (**Name**). For example, if a Heat Transfer in Fluids interface is included in the component, the **Temperature (ht)** option is available.

Absolute Pressure

This input appears when a material requires the absolute pressure as a model input. The absolute pressure is used to evaluate material properties, but it also relates to the value of the calculated pressure field. There are generally two ways to calculate the pressure when describing fluid flow: either to solve for the absolute pressure or for a pressure (often denoted gauge pressure) that relates to the absolute pressure through a reference pressure.

The choice of pressure variable depends on the system of equations being solved. For example, in a unidirectional incompressible flow problem, the pressure drop over the modeled domain is probably many orders of magnitude smaller than the atmospheric pressure, which, when included, may reduce the stability and convergence properties of the solver. In other cases, such as when the pressure is part of an expression for the gas volume or the diffusion coefficients, it may be more convenient to solve for the absolute pressure.

The default **Absolute pressure** p_A is $p + p_{\mathrm{ref}}$ where p is the dependent pressure variable from the Navier–Stokes equations, and p_{ref} is from the user input defined at the physics interface level. When p_{ref} is nonzero, the physics interface solves for a gauge pressure. If the pressure field instead is an absolute pressure field, p_{ref} should be set to 0.

The **Absolute pressure** field can be edited by clicking **Make All Model Inputs Editable** ( ) and entering the desired value in the input field.

FLUID PROPERTIES

If density variations with respect to pressure are to be included in the computations, the flow must be set to compressible.

The **Dynamic viscosity** μ describes the relationship between the shear rate and the shear stresses in a fluid. Intuitively, water and air have low viscosities, and substances often described as thick (such as oil) have higher viscosities.

LOCATION IN USER INTERFACE

Context Menus

Brinkman Equations > **Fluid Properties**

Ribbon

Physics tab with **Brinkman Equations** selected:

Domains > **Fluid Properties**

Gravity

The **Gravity** global feature is automatically added when **Include gravity** is selected at the interface level in the **Physical Model** settings. It defines the gravity forces from the **Acceleration of gravity** value. When a turbulence model that solves for the turbulent kinetic energy, k, is used, the option **Include buoyancy-induced turbulence** is available. When selected, the **Buoyancy contribution** is by default set to **Automatic from multiphysics**. Contributions are only obtained from multiphysics couplings that support buoyancy-induced turbulence, such as Nonisothermal Flow. If the **Buoyancy contribution** is switched to **User defined**, a text field for the **Turbulent Schmidt number** appears. See also Theory for Buoyancy-Induced Turbulence in the *CFD Module User's Guide*.

This feature requires a specific license. For a detailed overview of the functionality available in each product visit https://www.comsol.com/products/specifications/.

ACCELERATION OF GRAVITY

The **Acceleration of gravity** (SI unit m/s, default value $-g_{\text{const}}\mathbf{e_z}$ in 2D axial symmetry and 3D and $-g_{\text{const}}\mathbf{e_y}$ in 2D) is used to define the gravity forces. It should be a global quantity.

LOCATION IN USER INTERFACE

Context Menus

Brinkman Equations > **Gravity**

The Free and Porous Media Flow, Brinkman Interface

The **Free and Porous Media Flow, Brinkman (fp)** interface ( ) is found under the **Porous Media and Subsurface Flow** branch ( ) when adding a physics interface. It is used to compute fluid velocity and pressure fields of single-phase flow where free flow is connected to porous media. The Free and Porous Media Flow, Brinkman interface is used over at least two different domains: a free channel and a porous medium. The physics interface is well suited for transitions between slow flow in porous media, governed by the Brinkman equations, and fast flow in channels described by the Navier–Stokes equations. Fluids with varying density can be included at Mach numbers below 0.3. Also the viscosity of a fluid can vary, for example, to describe non-Newtonian fluids. The physics interface can be used for stationary and time-dependent analyses.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Fluid Properties**, **Wall**, and **Initial Values**. Then, from the **Physics** toolbar, add a **Porous Medium** node to be used on the domain selection corresponding to the porous media, or add other nodes that implement, for example, boundary conditions and volume forces. You can also right-click **Free and Porous Media Flow, Brinkman** to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `fp`.

PHYSICAL MODEL

Compressibility

By default the physics interface uses the **Incompressible flow** formulation of the Navier–Stokes and Brinkman equations to model constant density flow. If required, select

Weakly compressible flow from the **Compressibility** list, to account for small variations in the density, which are only dependent on the temperature (nonisothermal flow) or **Compressible flow (Ma<0.3)** for fully compressible flow. However, for the flow modeled with this physics interface, the Mach number must be below 0.3.

Swirl Flow

For 2D axisymmetric components, select the **Swirl flow** checkbox to include the swirl velocity component, that is the velocity component u_φ in the azimuthal direction. While u_φ can be nonzero, there can be no gradients in the φ direction. Note that this feature is only available for specific modules. Visit https://www.comsol.com/products/specifications/ for a detailed overview.

Neglect Inertial Term

Select the **Neglect inertial term (Stokes flow)** checkbox if the inertial forces are small compared to the viscous forces. This is typical for creeping flow, where $\mathrm{Re} << 1$.

Enable porous media domains

The **Enable porous media domains** checkbox is selected by default to solve the Brinkman equations in porous domains. If it is unchecked, the **Porous Medium** node is no longer available in this interface.

Include Gravity

Gravity is not included by default. Select the **Include gravity** checkbox to activate the acceleration of gravity. This automatically adds a global **Gravity** feature node to the interface model tree, and the buoyancy force is included in the Equations.

Also, when the **Include gravity** checkbox is selected, the **Use reduced pressure** option changes the pressure formulation from using the total pressure (default) to using the reduced pressure. This option is suitable for configurations where the density changes are very small; otherwise, the default formulation can be used. For more information, see Gravity.

Porous Treatment of No Slip Condition

Choose how the **No Slip** condition on internal boundaries should be treated. The options are **Standard no slip formulation** and **Porous slip** (default). The latter option provides a unified treatment when the porous matrix is fully resolved as well as when it is under resolved ensuring a smooth transition between regions with different resolutions; see No Slip under Wall in The Laminar Flow and Creeping Flow Interfaces section.

Reference Pressure Level

Enter a **Reference pressure level** p_{ref} (SI unit: Pa). The default value is `1[atm]`.

Reference Temperature

Enter a **Reference temperature** T_{ref} (SI unit: K). The default value is `293.15[K]`.

Reference Position

If **Include gravity** is selected, a **Reference position** r_{ref} (SI unit: m) can be specified which is then used for the calculation of the hydrostatic pressure.

TURBULENCE

Turbulent flow can be simulated by changing the **Turbulence model type** to **RANS-EVM** (Reynolds-Averaged Navier–Stokes, eddy-viscosity model), **RANS-RSM** (Reynolds-Averaged Navier–Stokes, Reynolds stress model), or **Large Eddy Simulation** (which is only available in 3D). If turbulent flow is activated, you can choose from different **Turbulence model**s and options for **Wall treatment**. For a description of the different turbulence models, wall treatment options, and turbulence model parameters, see Theory for the Turbulent Flow Interfaces in the *CFD Module User's Guide*.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface — the **Velocity field** $\mathbf{u}$ (SI unit: m/s) and its components, and the **Pressure** p (SI unit: Pa).

- Domain, Boundary, Point, and Pair Nodes for the Free and Porous Media Flow, Brinkman Interface
- Theory for the Free and Porous Media Flow, Brinkman Interface

Domain, Boundary, Point, and Pair Nodes for the Free and Porous Media Flow, Brinkman Interface

The Free and Porous Media Flow, Brinkman Interface has the following domain, boundary, point, and pair nodes, listed in alphabetical order, available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

- Fluid Properties
- Gravity
- Initial Values
- Porous Medium
- Mass Source
- Volume Force
- Wall

Note that some features are only available with certain COMSOL products (see https://www.comsol.com/products/specifications/).

The following nodes (listed in alphabetical order) are described for the Laminar Flow interface:

- No Viscous Stress
- Flow Continuity
- Inlet
- Line Mass Source
- Outlet
- Open Boundary
- Periodic Flow Condition
- Point Mass Source
- Pressure Point Constraint
- Symmetry

!	In the *COMSOL Multiphysics Reference Manual* see Table 2-4 for links to common sections and Table 2-5 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Fluid Properties

Use the **Fluid Properties** node to define the fluid material, density, and dynamic viscosity.

FLUID PROPERTIES

The default **Fluid material** uses the **Domain material** (the material defined for the domain). Select another material as needed.

The default **Density** ρ (SI unit: kg/m^3) uses values **From material** based on the **Fluid material** selection. For **User defined** enter another value or expression. The default is 0 kg/m^3.

The **Dynamic viscosity** μ (SI unit: Pa·s) uses values **From material** based on the **Fluid material** selection. For **User defined** enter another value or expression. The default is 0 Pa·s.

Porous Medium

The **Porous Medium** node adds the Brinkman equations (excluding any mass sources) to the interface. It has two default subfeatures — the Fluid subfeature where the fluid density ρ(SI unit: kg/m^3) and dynamic viscosity μ (SI unit: Pa·s) are defined and the Porous Matrix subfeature where the permeability κ (SI unit: m^2) and porosity ε_p (dimensionless) are specified.

FLOW MODEL

Define if the flow follows a linear or nonlinear pressure-velocity relationship.

- **Darcian flow** (default) defines a linear relationship characteristic for low Reynolds number laminar flows.
- **Non-Darcian flow** defines a nonlinear relationship due to inertial or turbulence effects.

POROUS MEDIUM TURBULENCE MODEL

Defines a model which complements the basic turbulence model and accounts for the influence of the porous matrix on turbulent flow in Porous Media.

- **Default** and **Nakayama-Kuwahara** specify **Coefficient of subgrid turbulence generation by porous matrix** C_{stpm} which by default is set to 0.212.
- **Pedras-de Lemos** asks to specify **Choice of the Pedras-de Lemos model coefficient**. When **User defined** is chosen, specify **Coefficient of subgrid turbulence generation by porous matrix** C_{stpm} with default value 0.212. Choosing **Original** results in $C_{stpm} = 0.28 \cdot \sqrt{\varepsilon_p}$, while choosing **Recalibrated** results in $C_{stpm} = 0.18$.

Fluid

This node defines the material properties of the fluid of the Porous Medium parent node.

MODEL INPUT

This section contains fields and values that are inputs for expressions defining material properties. If such user-defined property groups are added, the model inputs appear here.

FLUID PROPERTIES

Specify the **Density** ρ and the **Dynamic viscosity** μ (SI unit: Pa·s) of the fluid. The defaults use values **From material**, for **User defined** enter a value or expression.

The dynamic viscosity describes the relationship between the shear stresses and the shear rate in a fluid. Intuitively, water and air have a low viscosity, and substances often described as thick, such as oil, have a higher viscosity.

If the Polymer Flow Module license is available and for Darcian flow, also non-Newtonian models are available and the **Constitutive Relation** can be switched between **Specify dynamic viscosity** (default) or **Inelastic non-Newtonian**.

Constitutive Relation

Use the default option to either get the dynamic viscosity from a material, or to add a user defined expression. The default option lets you either use the dynamic viscosity from a material or define it with a custom expression. The **Inelastic non-Newtonian** option provides several models and defines the **Apparent shear rate**.

Inelastic Non-Newtonian

The following inelastic non-Newtonian Models are available for the **Fluid** feature under the **Porous Medium** feature:

- Power Law
- Carreau
- Carreau-Yasuda
- Cross
- Cross-Williamson
- Sisko

The setup of these models in porous media is similar to their definition under the Fluid Properties feature.

Apparent Shear Rate

To define the apparent shear rate $\dot{\gamma}_{\text{app}}$, either enter a user-defined expression for the correction factor (α) or choose the **Capillary bundle approach** from the list and provide a value for the Tortuosity factor (C).

	• Read more about the theory of Non-Newtonian Fluids in Porous Media in the *Polymer Flow Module User's Guide*

Porous Matrix

This node defines the porosity and material properties of the solid matrix of the Porous Medium parent node.

MODEL INPUT

This section contains fields and values that are inputs for expressions defining material properties. If such user-defined property groups are added, the model inputs appear here.

MATRIX PROPERTIES

The **Porosity** ε_p (a dimensionless number between 0 and 1) uses by default the value **From material**. For **User defined** the default value is 1 which is equivalent to free flow.

Select a **Permeability model** to specify the capacity of the porous material to transmit flow. Depending on the **Flow model** selection in the parent **Porous Medium** feature node you can choose between the following options:

- **Permeability** (the default) to directly enter the permeability of the porous matrix or **Kozeny-Carman** to define the permeability from the porosity and mean **Particle diameter** for **Darcian** flow or
- **Forchheimer** or **Ergun** for **Non-Darcian** flow.

Note that some of these options are only available for certain modules. For a detailed overview of the functionality available in each product, visit https://www.comsol.com/products/specifications/.

The default **Permeability** κ(SI unit: m^2) uses the value **From material**, as defined by the **Porous material** list. For **User defined** select **Isotropic** to define a scalar value or **Diagonal** or **Symmetric** to define a tensor value.

For **Kozeny-Carman**, enter the mean **Particle diameter** d_p (SI unit: m), the default value is 0.5 mm.

In case a **Non-Darcian** flow model is chosen in the parent node, **Forchheimer** is the default selection for the **Permeability model**. For **Forchheimer**, the default **Permeability** κ (SI unit: m^2) uses the value **From material**. Furthermore, the dimensionless **Forchheimer parameter** c_F can be defined. The default value is 0.55.

If **Ergun** is selected, enter the mean **Particle diameter** d_p (default value: 0.5 mm). The permeability κ is then calculated using Equation 2-4 in the *Porous Media Flow Module User's Guide*.

- About Darcian and Non-Darcian Flow in the *Porous Media Flow Module User's Guide*
- Permeability Models in the *Porous Media Flow Module User's Guide*

Mass Source

Enter a value or expression for an optional mass source (or sink) **Source term** Q_m (SI unit: $kg/(m^3 \cdot s)$). This term accounts for mass deposit or mass creation within porous domains. The physics interface assumes that the mass exchange occurs at zero velocity.

Volume Force

The **Volume Force** node specifies the force $\mathbf{F}$ on the right-hand side of the Navier–Stokes or Brinkman equations, depending on whether a Fluid Properties or Porous Medium node is active on the domain. It then acts on each fluid element in the specified domains.

VOLUME FORCE

Enter the components of the **Volume force** $\mathbf{F}$ (SI unit: N/m^3).

Initial Values

The **Initial Values** node adds initial values for the velocity field and the pressure that can serve as an initial condition for a transient simulation or as an initial guess for a nonlinear solver.

INITIAL VALUES

Enter initial values or expressions for the **Velocity field** $\mathbf{u}$ (SI unit: m/s) and for the **Pressure** p (SI unit: Pa). The default values are 0 m/s and 0 Pa, respectively.

Gravity

The **Gravity** global feature is automatically added when **Include gravity** is selected at the interface level in the **Physical Model** settings. It defines the gravity forces from the **Acceleration of gravity** value. When a turbulence model that solves for the turbulent kinetic energy, k, is used, the option **Include buoyancy-induced turbulence** is available. When selected, the **Buoyancy contribution** is by default set to **Automatic from multiphysics**. Contributions are only obtained from multiphysics couplings that support buoyancy-induced turbulence, such as Nonisothermal Flow. If the **Buoyancy contribution** is switched to **User defined**, a text field for the **Turbulent Schmidt number** appears. See also Theory for Buoyancy-Induced Turbulence in the *CFD Module User's Guide*.

This feature requires a specific license. For a detailed overview of the functionality available in each product visit https://www.comsol.com/products/specifications/.

ACCELERATION OF GRAVITY

The **Acceleration of gravity** (SI unit m/s, default value $-g_{\text{const}}\mathbf{e_z}$ in 2D axial symmetry and 3D and $-g_{\text{const}}\mathbf{e_y}$ in 2D) is used to define the gravity forces. It should be a global quantity.

Microfluidic Wall Conditions

Use the **Microfluidic Wall Conditions** node to add boundary conditions to the moving wall and specify whether to use viscous slip or thermal creep.

BOUNDARY CONDITION

The default **Boundary condition** for the wall is **Slip velocity**. Enter values or expressions for the components of the **Velocity of moving wall** $\mathbf{u}_{\text{w}}$ (SI unit: m/s).

Use Viscous Slip

Select the **Use viscous slip** checkbox to define the slip length:

- The default is **User defined**. Enter a value for L_s (SI unit: m). The default is 1e-7 m.
- Select **Maxwell's model** to calculate it from:

$$L_s = \left(\frac{2-\alpha_v}{\alpha_v}\right)\lambda$$

- Then enter values or expressions for the **Tangential momentum accommodation coefficient** (TMAC) α_v (dimensionless) (the default is 0.9) and the **Mean free path** λ (SI unit: m) (the default is 1e-6 m).

Use Thermal Creep

Select the **Use thermal creep** checkbox to activate the thermal creep component of the boundary condition. Enter the fluid's **Temperature** T (SI unit: K) and the **Thermal slip coefficient** σ_T. The default temperature is 293.15 K and the default thermal slip coefficient is 0.75.

If you also have a license for the MEMS Module, an additional **Boundary condition** option **Electroosmotic velocity** is available. This is described in the *MEMS Module User's Guide*.

Wall

The **Wall** node includes a set of boundary conditions describing fluid-flow conditions at stationary, moving, and leaking walls.

BOUNDARY CONDITION

Select a **Boundary condition** for the wall.

- No Slip[1]
- Slip
- Leaking Wall

No Slip

No slip is the default boundary condition for a stationary solid wall for laminar flow (and SST, Low Re k-ε, Algebraic yPlus, L-VEL, and Spalart–Allmaras turbulence models). The condition prescribes $\mathbf{u} = 0$; that is, the fluid at the wall is not moving.

Slip

The **Slip** option prescribes a no-penetration condition, $\mathbf{u}\cdot\mathbf{n} = 0$. It is implicitly assumed that there are no viscous effects at the slip wall and hence, no boundary layer develops. From a modeling point of view, this can be a reasonable approximation if the main effect of the wall is to prevent fluid from leaving the domain.

Leaking Wall

This boundary condition can be used to simulate a wall where fluid is leaking into or leaving the domain with the velocity $\mathbf{u} = \mathbf{u}_l$ through a perforated wall. The components of the **Fluid velocity** $\mathbf{u}_l$ on the leaking wall should be specified.

CONSTRAINT SETTINGS

This section is displayed by clicking the **Show** button ( ) and selecting **Advanced Physics Options**.

	• Theory for the Wall Boundary Condition • The Moving Mesh Interface in the *COMSOL Multiphysics Reference Manual*

The Free and Porous Media Flow, Darcy Interface

The **Free and Porous Media Flow, Darcy** interface ( ) combines the **Darcy's Law** and **Laminar Flow** interfaces to compute fluid velocity and pressure fields where free flow is connected to porous media. The physics interface is suited for situations when both the free flow and the flow in the porous media are laminar.

When a predefined **Free and Porous Media Flow, Darcy** interface is added from the **Porous Media and Subsurface Flow** branch ( ) of the **Model Wizard** or **Add Physics** window, the **Darcy's Law** and **Laminar Flow** interfaces are added to the Model Builder. In addition, the **Multiphysics** node is added, which automatically includes the **Free and Porous Media Flow Coupling** multiphysics coupling.

On the Constituent Physics Interfaces

The **Darcy's Law** interface is used to simulate fluid flow through interstices in a porous medium. It can be used to model low-velocity flows in media where the permeability and porosity are very small, and for which the pressure gradient is the major driving force and the flow is mostly influenced by the frictional resistance within the pores.

The **Laminar Flow** interface is used to compute the velocity and pressure for a fluid flow in the laminar flow regime. A flow will remain laminar as long as the Reynolds number is below a certain critical value. At higher Reynolds numbers, disturbances have a tendency to grow and cause transition to turbulence.

SETTINGS FOR PHYSICS INTERFACES AND COUPLING FEATURES

When physics interfaces are added using the predefined couplings, for example **Free and Porous Media Flow, Darcy**, specific settings are included with the physics interfaces and the coupling features.

However, if physics interfaces are added one at a time, followed by the coupling features, these modified settings are not automatically included.

Free and Porous Media Flow Coupling (Multiphysics Coupling)

The **Free and Porous Media Flow Coupling** multiphysics coupling node ( ) bidirectionally links the **Laminar Flow** and **Darcy's Law** interfaces.

SETTINGS

The **Label** is the default multiphysics coupling feature name.

The **Name** is used primarily as a scope prefix for variables defined by the coupling node. Refer to such variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different coupling nodes or physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first multiphysics coupling feature in the model) is `nsd1`.

DOMAIN SELECTION

When nodes are added from the context menu, you can select **Manual** (the default) from the **Selection** list to choose specific domains to define the multiphase flow coupling, or select **All domains** as needed.

When the **Free and Porous Media Flow Coupling** is added as an effect of adding a Free and Porous Media Flow, Darcy multiphysics interface, the selection is the intersection of the boundaries of the participating physics interfaces.

Only boundaries that are active in the participating physics interfaces (which are chosen from the **Coupled Interfaces** selection list) can be selected.

COUPLED INTERFACES

This section defines the physics involved in the multiphysics coupling. The **Free flow** and **Porous media flow** lists include all applicable physics interfaces.

The default values depend on how the coupling node is created.

- If it is added from the **Physics** ribbon (Windows users), **Physics** contextual toolbar (Mac and Linux users), or context menu (all users), then the first physics interface of each type in the component is selected as the default.
- If it is added automatically when a multiphysics interface is selected in the **Model Wizard** or **Add Physics** window, then the two participating physics interfaces are selected.

You can also select **None** from either list to uncouple the Free and Porous Media Flow Coupling node from a physics interface. If the physics interface is removed from the **Model Builder**, for example **Darcy's Law** is deleted, then the **Porous media flow** list defaults to **None** as there is nothing to couple to.

COUPLING SETTINGS

This section defines the settings for the **Free flow boundary condition**.

- When **No slip** is selected, the tangential component of the fluid velocity at the free-porous interface on the free-flow side (computed in the **Free flow** interface) is set to zero.
- When **Continuous tangential velocity** is selected, the tangential velocity component of the flow on both sides of the free-porous interface is continuous. In addition, continuity of normal stresses and conservation of mass across the interface are ensured.
- When **Beavers-Joseph** is selected, the difference of the tangential velocity components of the flow on both sides of the free-porous interface is proportional to the shear stress at the free-porous interface on the free-flow side. For this option, enter a value or expression for the **Beavers and Joseph parameter** a_{BJ} (dimensionless) that determines the proportionality. In addition, select the checkbox **Use projected permeability** to use only the component of the permeability tensor in the direction of the difference of the tangential velocities on both sides of the interface, instead of the trace of the permeability tensor, in determining the proportionality.
- When **Beavers-Joseph-Saffman** is selected, the tangential velocity component of the flow at the free-porous interface on the free-flow side is proportional to the shear stress at the interface on the free-flow side. For this option also, enter a value or expression for the **Beavers and Joseph parameter** a_{BJ} (dimensionless) that determines the proportionality. In addition, select the checkbox **Use projected permeability** to use only the component of the permeability tensor in the direction of the difference of the tangential velocities on both sides of the interface, instead of the trace of the permeability tensor, in determining the proportionality.
- When **Viscous slip** is selected, the difference of the tangential velocity components of the flow on the free-flow side and a user-supplied interfacial velocity is proportional to the shear stress at the free-porous interface on the free-flow side. Enter values for the **Slip length** L_s (SI unit: m, the default is 1e-7 m), and an **Interfacial velocity** $\mathbf{u}_\mathrm{b}$ (SI unit: m/s, the default is 0 m/s).

In all the above cases, additionally continuity of normal stresses and conservation of mass across the interface are ensured.

	Please find related information in the *CFD Module User's Guide*: • The Darcy's Law Interface • Theory for the Darcy's Law Interface • The Laminar Flow Interface • Theory for the Single-Phase Flow Interfaces • Theory for the Free and Porous Media Flow, Darcy Interface

Theory for the Darcy's Law Interface

The Darcy's Law Interface theory is described in this section:

- About Darcy's Law
- Darcy's Law — Equation Formulation
- Storage Models
- Average Linear Velocity
- Dual Porosity and Dual Permeability Theory
- References for the Darcy's Law Interface

About Darcy's Law

In a porous medium, the global transport of momentum by shear stresses in the fluid is often negligible, because the pore walls impede momentum transport to the fluid outside the individual pores. A detailed description, down to the resolution of every pore, is not practical in most applications. A homogenization of the porous and fluid media into a single medium is a common alternative approach. Darcy's law together with the continuity equation and equation of state for the pore fluid (or gas) provide a complete mathematical model suitable for a wide variety of applications involving porous media flows, for which the pressure gradient is the major driving force.

Darcy's law describes fluid movement through interstices in a porous medium. Because the fluid loses considerable energy to frictional resistance within pores, flow velocities in porous media are very low. The Darcy's Law interface can be applied to small-scale tasks in chemical engineering as well as to large-scale geophysical or hydrological tasks such as water moving in an aquifer or stream bank, oil migrating to a well, and even magma rising through the earth to a chamber in a volcano (see Ref. 1, Ref. 2, Ref. 3, and Ref. 4). Also set up multiple Darcy's Law interfaces to model multiphase flows involving more than one mobile phase.

Darcy's law describes flow in porous media driven by gradients in the hydraulic potential field, which has units of pressure. For many applications it is convenient to represent the total hydraulic potential or the pressure and the gravitational components with equivalent heights of fluid or head. Division of potential by the fluid weight can simplify modeling because units of length make it straightforward to compare to many physical data. Consider, for example, fluid levels in wells, stream heights, topography, and velocities. The physics interface also supports specifying

boundary conditions and result evaluation using hydraulic head and pressure head. In the physics interface, pressure is always the dependent variable.

Darcy's Law — Equation Formulation

Darcy's law states that the velocity field is determined by the pressure gradient, the fluid viscosity, and the structure of the porous medium:

$$\mathbf{u} = -\frac{\kappa}{\mu}\nabla p \tag{6-20}$$

In this equation, $\mathbf{u}$ is the Darcy's velocity or specific discharge vector (SI unit: m/s); κ is the permeability of the porous medium (SI unit: m^2); μ is the fluid's dynamic viscosity (SI unit: Pa·s); p is the pore pressure (SI unit: Pa) and ρ is the density of the fluid (SI unit: kg/m^3).

- The above equation formulation is called linear Darcy's law. The applicability of this formulation is discussed in the chapter About Darcian and Non-Darcian Flow in the *Porous Media Flow Module User's Guide*.
- Permeability can be defined in different ways, either directly or based on predefined permeability models. These are described in detail in the chapter Permeability Models.
- For a detailed overview of the permeability models available in each product visit https://www.comsol.com/products/specifications/.

The Darcy's Law interface combines Darcy's law with the continuity equation

$$\frac{\partial}{\partial t}(\rho\varepsilon_p) + \nabla\cdot(\rho\mathbf{u}) = Q_m \tag{6-21}$$

In the above equation, ρ is the fluid density (SI unit: kg/m^3), ε_p is the porosity, and Q_m is a mass source term (SI unit: $kg/(m^3\cdot s)$). Porosity is defined as the fraction of the control volume that is occupied by pores. Thus, the porosity can vary from zero for pure solid regions to unity for domains of free flow.

For large-scale applications it might be necessary to take gravity effects into account. Darcy's law then applies when the gradient in hydraulic potential drives fluid movement in the porous medium. Darcy's law then has the form:

$$\mathbf{u} = -\frac{\kappa}{\mu}(\nabla p - \rho \mathbf{g}) \tag{6-22}$$

- See the section Gravity Effects in the *Subsurface Flow Module User's Guide*.
- Note that gravity effects are only included in some modules. For a detailed overview of the functionality available in each product visit https://www.comsol.com/products/specifications/.
- Gravity effects are not active by default. Select the checkbox **Include gravity** to activate the acceleration of gravity. Setting the elevation D to zero also turns off gravity effects.

Storage Models

The continuity equation (Equation 6-21) allows flexible specification of relationships between parameters like density or permeability with respect to variables such as pressure, temperature, concentration, and more.

Expanding the time-derivative term and defining the porosity and density as functions of the pressure and using the chain rule results in

$$\frac{\partial}{\partial t}(\rho \varepsilon_p) = \varepsilon_p \frac{\partial \rho}{\partial t} + \rho \frac{\partial \varepsilon_p}{\partial t} = \varepsilon_p \frac{\partial \rho}{\partial p}\frac{\partial p}{\partial t} + \rho \frac{\partial \varepsilon_p}{\partial p}\frac{\partial p}{\partial t}$$

By inserting the definition of fluid compressibility $\chi_f = (1/\rho)(\partial\rho/\partial p)$ to the right-hand side and rearrange the following expression is obtained

$$\frac{\partial(\rho \varepsilon_p)}{\partial t} = \rho\left(\varepsilon_p \chi_f + \frac{\partial \varepsilon_p}{\partial p}\right)\frac{\partial p}{\partial t} = \rho S_p \frac{\partial p}{\partial t}$$

Using this relation, the generalized governing equation (Equation 6-21) takes the following form:

$$\rho S_p \frac{\partial p}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = Q_m \tag{6-23}$$

In this equation, S_p is the storage coefficient (SI unit: 1/Pa), which can be interpreted as the weighted compressibility of the porous material and the fluid. The storage can be an expression involving results from a solid-deformation equation or an expression involving temperatures and concentrations from other analyses. The Darcy's Law

interface implements Equation 6-23 in the **Porous Medium** node, which explicitly includes different storage models to choose from:

- **From density and porosity**, where the storage directly depends on changes in porosity or fluid density
- **Linearized storage**, which defines S_p using the compressibility of the fluid χ_f and of the porous matrix χ_p according to

$$S_p = \varepsilon_p \chi_f + (1 - \varepsilon_p)\chi_p$$

- **Poroelastic storage** where

$$S_p = \varepsilon_p \chi_f .$$

	Storage models are only available for the Subsurface Flow Module and the Porous Media Flow Module. For a detailed overview of the functionality available in each product visit https://www.comsol.com/products/specifications/.

Average Linear Velocity

Because fluids typically occupy only 10% to 50% of a porous medium, it follows that velocities within the pore channels exceed the Darcy velocity, $\mathbf{u}$, on the order of two to ten times. For clarity, the physics interface includes the average linear velocity within the pores, $\mathbf{u}_\alpha$, (also termed the seepage velocity) defined as $\mathbf{u}_\alpha = \mathbf{u}/\varepsilon_p$, where ε_p is the porosity.

Dual Porosity and Dual Permeability Theory

The first well known publication on this topic is "The Behavior of Naturally Fractured Reservoirs" by J.E. Warren and P.J. Root from 1963. Since then the researchers further developed the idea of a dual porosity/permeability type of a porous medium. One of the well established models is based on the findings of H. Gerke and M. van Genuchten (Ref. 9). Basically the idea behind is to solve for each part of the porous medium (macro- and micropores) the relevant equations and connect them via an exchange term.

DUAL POROSITY MEDIUM

Darcy's Law is solved for the macropores and taking into account their volume fraction θ_M the equation reads:

$$\theta_M\left(\rho S_{\mathrm{p,M}}\frac{\partial p_{\mathrm{M}}}{\partial t}+\nabla(\rho\mathbf{u}_{\mathrm{M}})\right) = \theta_{\mathrm{M}}Q_{\mathrm{M}}-Q_{\mathrm{ip}} \tag{6-24}$$

The term Q_{ip} describes the mass source from the Interporosity Flow which is the mass transfer from the macropores to the micropores system. An additional ODE for the (passive) micropores is solved which only act as additional storage volume:

$$(1-\theta_M)\left(\rho S_{\mathrm{p,m}}\frac{\partial p_{\mathrm{m}}}{\partial t}\right) = (1-\theta_{\mathrm{M}})Q_{\mathrm{M}}+Q_{\mathrm{ip}}\,.$$

The indices M and m stand for macropores and micropores, respectively.

DUAL PERMEABILITY MEDIUM

Darcy's law has to be solved for both the macroscale system and the microscale system:

$$\begin{gathered}\theta_{\mathrm{M}}\left(\frac{\partial}{\partial t}(\varepsilon_{\mathrm{p,M}}\rho)+\nabla\cdot(\rho\mathbf{u}_{\mathrm{M}})\right) = -Q_{\mathrm{ip}}+\theta_{\mathrm{M}}Q_{\mathrm{m}}\\ (1-\theta_{\mathrm{M}})\left(\frac{\partial}{\partial t}(\varepsilon_{\mathrm{p,m}}\rho)+\nabla\cdot(\rho\mathbf{u}_{\mathrm{m}})\right) = Q_{\mathrm{ip}}+(1-\theta_{\mathrm{M}})Q_{\mathrm{m}}\\ p = \theta_{\mathrm{M}}p_{\mathrm{M}}+(1-\theta_{\mathrm{M}})p_{\mathrm{m}}\end{gathered} \tag{6-25}$$

θ_{M} is the volume fraction of the macropores, Q_{ip} denotes the interporosity flow, signifying the mass transfer from the macropores (identified by index M) to the micropores (identified by index m).

Solving Darcy's law for both systems entails solving two equations, each associated with dependent pressure variables p_{m} and p_{M}. These equations are coupled via Q_{ip}. From this, average quantities for the dual permeability medium as a whole are computed. The average pressure of the dual permeability medium is defined as:

$$p = \theta_{\mathrm{M}}p_{\mathrm{M}}+(1-\theta_{\mathrm{M}})p_m$$

Likewise, average values for permeability, storage, velocity and other relevant parameters are computed.

UNSATURATED DUAL PERMEABILITY MEDIUM

Use the **Unsaturated Dual Permeability Medium** feature to model the transport in an unsaturated dual permeability medium where Richards' Equation (Equation 4-26) describes the transport in each system.

$$\theta_M\left(\rho\left(S_{e,M}S_{p,M}+\frac{C_{m,M}}{\rho g}\right)\frac{\partial p_M}{\partial t}+\nabla(\rho\mathbf{u}_M)\right)=-Q_{ip}+\theta_M Q_m$$
$$(1-\theta_M)\left(\rho\left(S_{e,m}S_{p,m}+\frac{C_{m,m}}{\rho g}\right)\frac{\partial p_m}{\partial t}+\nabla(\rho\mathbf{u}_m)\right)=Q_{ip}+(1-\theta_M)Q_m \tag{6-26}$$
$$p=\theta_M p_M+(1-\theta_M)p_m$$

θ_M is the volume fraction of the macropores, Q_{ip} is the interporosity flow which is the mass transfer from the macroscale to the microscale system. The indices M and m stand for macropores and micropores, respectively.

INTERPOROSITY FLOW

Specify the **Fluid Transfer Function** α_w which is used to calculate the interporosity flow, which is the mass exchange between macro- and microscale system:

$$Q_{ip}=\alpha_w(p_M-p_m) \tag{6-27}$$

with p_M being the pressure within the macroscale system and p_m the pressure within the microscale system

References for the Darcy's Law Interface

1. J. Bear, *Hydraulics of Groundwater*, McGraw Hill, 1979.

2. S.E. Ingebritsen and W.E. Sanford, *Groundwater in Geologic Processes*, Cambridge University Press, 1998.

3. N.H. Sleep and K. Fujita, *Principles of Geophysics*, Blackwell Science, 1997.

4. D.L. Turcotte and G. Schubert, *Geodynamics*, Cambridge University Press, 2002.

5. J. Bear, *Dynamics of Fluids in Porous Media*, Elsevier Scientific Publishing, 1972.

6. Ö. Akgiray and A.M. Saatçı, "A New Look at Filter Backwash Hydraulics," *Water Sci. Technol. Water Supply*, vol. 1, no. 2, pp. 65–72, 2001.

7. L. Klinkenberg, "The permeability of porous media to liquids and gases," *Drilling and Production Practice*, Am. Petroleum Inst., pp. 200–213, 1941.

8. Yu-Shu Wu and others, "Gas Flow in Porous Media with Klinkenberg Effects," *Transp. Porous Media*, vol. 32, pp. 117–137, 1998.

9. H. Gerke and M. van Genuchten, "A dual-porosity model for simulating the preferential movement of water and solutes in structured porous media," *Water Resour. Res.*, vol. 29. pp. 305–319. 1993.

Theory for the Brinkman Equations Interface

The Brinkman Equations Interface theory is described in this section:

- About the Brinkman Equations
- Brinkman Equations Theory
- References for the Brinkman Equations Interface

About the Brinkman Equations

The ***Brinkman equations*** describe fluids in porous media for which the momentum transport within the fluid due to shear stresses is of importance. This mathematical model extends Darcy's law to include a term that accounts for the viscous transport in the momentum balance, and it treats both the pressure and the flow velocity vector as independent variables. Use the Free and Porous Media Flow, Brinkman interface to model combinations of porous media and free flow domains. These types of problems are often encountered in applications such as monolithic reactors and fuel cells.

The Free and Porous Media Flow, Brinkman Interface

In porous domains, the flow variables and fluid properties are defined at any point inside the medium by means of averaging of the actual variables and properties over a certain volume surrounding the point. This control volume must be small compared to the typical macroscopic dimensions of the problem, but it must be large enough to contain many pores and solid matrix elements.

Porosity is defined as the fraction of the control volume that is occupied by pores. Thus, the porosity can vary from zero for pure solid regions to unity for domains of free flow.

The physical properties of the fluid, such as density and viscosity, are defined as *intrinsic volume averages* that correspond to a unit volume of the pores. Defined this way, they present the relevant physical parameters that can be measured experimentally, and they are assumed to be continuous with the corresponding parameters in the adjacent free flow.

The flow velocity is defined as a *superficial volume average*, and it corresponds to a unit volume of the medium including both the pores and the matrix. It is sometimes called the Darcy velocity, defined as the volume flow rate per unit cross section of the medium. Such a definition makes the velocity field continuous across the boundaries between porous regions and regions of free flow.

Brinkman Equations Theory

The dependent variables in the Brinkman equations are the Darcy velocity and the pressure. The flow in porous media is governed by a combination of the continuity equation and the momentum equation, which together form the Brinkman equations:

$$\frac{\partial}{\partial t}(\varepsilon_p \rho) + \nabla \cdot (\rho \mathbf{u}) = Q_m \tag{6-28}$$

$$\begin{aligned} &\frac{\rho}{\varepsilon_p}\left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\frac{\mathbf{u}}{\varepsilon_p}\right) = \\ &-\nabla p + \nabla \cdot \left[\frac{1}{\varepsilon_p}\left\{\mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I}\right\}\right] - \left(\kappa^{-1}\mu + \frac{Q_m}{\varepsilon_p^2}\right)\mathbf{u} + \mathbf{F} \end{aligned} \tag{6-29}$$

In these equations:

- μ (SI unit: kg/(m·s)) is the dynamic viscosity of the fluid
- $\mathbf{u}$ (SI unit: m/s) is the velocity vector
- ρ (SI unit: kg/m^3) is the density of the fluid
- p (SI unit: Pa) is the pressure
- ε_p is the porosity
- κ (SI unit: m^2) is the permeability of the porous medium, and
- Q_m (SI unit: kg/(m^3·s)) is a mass source or sink

Influence of gravity and other volume forces can be accounted for via the force term $\mathbf{F}$ (SI unit: kg/(m^2·s^2)).

When the **Neglect inertial term (Stokes flow)** checkbox is selected, the term $(\mathbf{u} \cdot \nabla)(\mathbf{u}/\varepsilon_p)$ on the left-hand side of Equation 6-29 is disabled.

The mass source, Q_m, accounts for mass deposit and mass creation within the domains. The mass exchange is assumed to occur at zero velocity.

The Forchheimer and Ergun drag options add a viscous force proportional to the square of the fluid velocity, $\mathbf{F} = -\rho\beta|\mathbf{u}|\mathbf{u}$, on the right-hand side of Equation 6-29; see References for the Darcy's Law Interface for details.

In case of a flow with variable density, Equation 6-28 and Equation 6-29 must be solved together with the equation of state that relates the density to the temperature and pressure (for instance the ideal gas law).

For incompressible flow, the density stays constant in any fluid particle, which can be expressed as

$$\frac{\partial}{\partial t}(\varepsilon_p \rho) + \mathbf{u} \cdot \nabla \rho = 0$$

and the continuity equation (Equation 6-28) reduces to

$$\rho \nabla \cdot \mathbf{u} = Q_m$$

References for the Brinkman Equations Interface

1. D. Nield and A. Bejan, *Convection in Porous Media*, 3rd ed., Springer, 2006.

2. M. Le Bars and M.G. Worster, "Interfacial Conditions Between a Pure Fluid and a Porous Medium: Implications for Binary Alloy Solidification," *J. Fluid Mech.*, vol. 550, pp. 149–173, 2006.

Theory for the Free and Porous Media Flow, Brinkman Interface

The Free and Porous Media Flow, Brinkman Interface uses the Navier–Stokes equations to describe the flow in open regions, and the Brinkman equations to describe the flow in porous regions.

The same fields, $\mathbf{u}$ and p, are solved for in both the free flow domains and in the porous domains. This means that the pressure in the free fluid and the pressure in the pores is continuous over the interface between a free flow domain and a porous domain. It also means that continuity is enforced between the fluid velocity in the free flow and the Darcy velocity in the porous domain. This treatment is one of several possible models for the physics at the interface. Examples of other models can be found in Ref. 1.

The continuity in $\mathbf{u}$ and p implies a stress discontinuity at the interface between a free-flow domain and a porous domain. The difference corresponds to the stress absorbed by the rigid porous matrix, which is a consequence implicit in the formulations of the Navier–Stokes and Brinkman equations.

Reference for the Free and Porous Media Flow, Brinkman Interface

1. M.L. Bars and M.G. Worster, "Interfacial Conditions Between a Pure Fluid and a Porous Medium: Implications for Binary Alloy Solidification," *J. Fluid Mech.*, vol. 550, pp. 149–173, 2006.

Theory for the Free and Porous Media Flow, Darcy Interface

The **Free and Porous Media Flow, Darcy** interface uses the Navier–Stokes equations to describe the flow in the free-flow region, implemented by the coupled Laminar Flow interface, and Darcy's law, implemented by the coupled Darcy's Law interface, to describe the flow in the porous region.

In the free-flow region, the velocity u and pressure p are solved for, whereas in the porous region only the pressure p is solved for, and the velocity is calculated from the pressure by Darcy's law.

The coupling between the free and porous medium flow, implemented by the Free and Porous Media Flow Coupling, ensures conservation of mass across the free-porous interface, which is enforced by the condition

$$\mathbf{n} \cdot (\rho_{\mathrm{ns}} \mathbf{u}_{\mathrm{ns}}) = \mathbf{n} \cdot (\rho_{\mathrm{d}} \mathbf{u}_{\mathrm{d}}) \tag{6-30}$$

Here ρ_{ns} and $\mathbf{u}_{\mathrm{ns}}$ are the density and velocity on the free-flow side of the interface, ρ_{d} and $\mathbf{u}_{\mathrm{d}}$ the density and velocity on the porous side, and $\mathbf{n}$ is a vector normal to the interface. In addition the coupling enforces the balance of the normal forces by:

$$p_{\mathrm{ns}} - \mathbf{n} \cdot \mathbf{K}\mathbf{n} = p_{\mathrm{d}} \tag{6-31}$$

where p_{ns} and p_{d} are the pressure on the free-flow side and porous side of the interface, respectively, and $\mathbf{K}$ is the viscous stress tensor (defined only on the free-flow side).

For the coupling condition for the tangential velocity component, there are several options. One of the most widely used conditions is the **Beavers-Joseph** interface condition (Ref. 1):

$$(\mathbf{I} - \mathbf{n} \otimes \mathbf{n})(\mathbf{u}_{\mathrm{ns}} - \mathbf{u}_{\mathrm{d}}) = \frac{\sqrt{\mathrm{tr}(\kappa)/n}}{\mu_{\mathrm{ns}} \alpha_{BJ}} (\mathbf{I} - \mathbf{n} \otimes \mathbf{n}) \mathbf{K}\mathbf{n} \tag{6-32}$$

where a_{BJ} is the Beavers and Joseph parameter, κ is the permeability tensor of the porous medium (defined on the porous side of the interface), μ_{ns} is the fluid's dynamic viscosity on the free-flow side of the interface, and n is the number of space dimensions.

When the velocity in the porous domain is much smaller than the velocity in the free flow, one can use a modification of the Beavers–Joseph condition which is given by the **Beavers–Joseph–Saffman** interface condition (Ref. 2):

$$(\mathbf{I}-\mathbf{n}\otimes\mathbf{n})\mathbf{u}_{\mathrm{ns}} = \frac{\sqrt{\mathrm{tr}(\kappa)/n}}{\mu_{\mathrm{ns}}\alpha_{BJ}}(\mathbf{I}-\mathbf{n}\otimes\mathbf{n})\mathbf{K}\mathbf{n} \tag{6-33}$$

For cases when the permeability tensor is not isotropic, the **Use projected permeability** option allows to take into account only the permeability in the direction of the tangential velocity component. This is accomplished by replacing the $\sqrt{\mathrm{tr}(\kappa)/n}$ term on the rights hand side of Equation 6-32 and Equation 6-33 by:

$$\sqrt{\mathbf{t}\cdot\kappa\mathbf{t}} \tag{6-34}$$

with $\mathbf{t}$ a unit vector tangent to the interface for 2D and 2D-axisymmetric cases, and for 3D cases by:

$$\sqrt{\mathbf{v}\cdot\kappa\mathbf{v}} \tag{6-35}$$

with $\mathbf{v}$ given by:

$$\mathbf{v} = \frac{(\mathbf{I}-\mathbf{n}\otimes\mathbf{n})\mathbf{K}\mathbf{n}}{\|(\mathbf{I}-\mathbf{n}\otimes\mathbf{n})\mathbf{K}\mathbf{n}\|} \tag{6-36}$$

If one considers the limit of the Beavers–Joseph condition for large values of the Beavers and Joseph parameter α_{BJ}, one obtains the **Continuous tangential velocity** condition:

$$(\mathbf{I}-\mathbf{n}\otimes\mathbf{n})(\mathbf{u}_{\mathrm{ns}}-\mathbf{u}_{\mathrm{d}}) = 0 \tag{6-37}$$

The same limit for the Beavers–Joseph–Saffman condition results in the **No slip** condition:

$$(\mathbf{I}-\mathbf{n}\otimes\mathbf{n})\mathbf{u}_{\mathrm{ns}} = 0 \tag{6-38}$$

The **Viscous slip** condition allows for a more general coupling condition. This interface condition is given by:

$$(\mathbf{I}-\mathbf{n}\otimes\mathbf{n})(\mathbf{u}_{\mathrm{ns}}-\mathbf{u}_{\mathrm{b}}) = \frac{L_s}{\mu_{\mathrm{ns}}}(\mathbf{I}-\mathbf{n}\otimes\mathbf{n})\mathbf{K}\mathbf{n} \tag{6-39}$$

Here L_s is a slip length, and $\mathbf{u}_b$ a user-defined interfacial velocity.

	Please find related information in the *CFD Module User's Guide*: • The Darcy's Law Interface • The Thin-Film and Porous Media Flow Interface • The Laminar Flow Interface • Theory for the Single-Phase Flow Interfaces

References

1. G.S. Beavers and D.D. Joseph, "Boundary Conditions at a Naturally Permeable Wall," *J. Fluid Mech.*, vol. 30, 1967.

2. P.G. Saffman, "On the Boundary Condition at the Surface of a Porous Medium," *Stud. Appl. Math.*, vol. 50, no. 2, pp. 93–101, 1971.

7

Rarefied Flow Interface

This chapter describes the physics interface available to model the flow of rarefied gases. The physics interface is found under the **Fluid Flow** > **Rarefied Flow** branch ( ). See Modeling Microfluidic Fluid Flows to help select the physics interface to use.

- The Slip Flow Interface
- Theory for the Slip Flow Interface

The Slip Flow Interface

The **Slip Flow (slpf)** interface ( ), found under the **Rarefied Flow** branch ( ) when adding a physics interface, is used to model thermal and isothermal flows within the slip-flow regime. In the slip-flow regime, the Navier–Stokes equations can be used to model the flow of the gas, except within a thin layer of rarefied gas adjacent to the walls (known as the Knudsen layer). The effect of the Knudsen layer on the continuum part of the flow can be modeled by means of modified boundary conditions for the Navier–Stokes equations. Thermal effects are also important in this regime, with effects such as thermal creep or transpiration often playing a significant role. For this reason the Slip Flow interface includes the heat flow equations. Typically slip flow applies at Knudsen numbers between 0.01 and 0.1.

When this physics interface is added, these default nodes are also added to the **Model Builder**: **Fluid**, **External Slip Wall**, and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and volume forces. You can also right-click **Slip Flow** to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `slpf`.

PHYSICAL MODEL

Select the **Neglect inertial term (Stokes flow)** checkbox to model flow at very low Reynolds numbers where the inertial term in the Navier–Stokes equations can be neglected. When this option is checked COMSOL Multiphysics solves the linear Stokes equations for the fluid flow. The *Stokes flow* or *creeping flow* regime frequently

applies in microfluidic devices, where the flow length scales are very small. Enter a **Reference pressure level** p_{ref}. The default value is `1[atm]`.

If you have the Heat Transfer Module, an additional checkbox is available for the modeling of heat transfer in biological tissue. See the *Heat Transfer Module User's Guide for information*.

DEPENDENT VARIABLES

This physics interface defines these dependent variables (fields):

- **Temperature** T (SI unit: K)
- **Velocity field** u (SI unit: m/s)
- **Pressure** p (SI unit: Pa)

For each of the dependent variables, the name can be changed in the corresponding field, but the name of fields and dependent variables must be unique within a model.

ADVANCED SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options**. Normally these settings do not need to be changed. The **Default model** is **Fluid**.

Select the **Use pseudo time stepping for stationary equation form** checkbox to add pseudo time derivatives to the equation when the **Stationary equation** form is used. When selected, also choose a **CFL number expression** — **Automatic** (the default) or **Manual**. **Automatic** calculates the local CFL number (from the Courant–Friedrichs–Lewy condition) from a built-in expression. For **Manual** enter a **Local CFL number** CFL_{loc}.

By default the **Enable conversions between material and spatial frames** checkbox is selected.

In the *COMSOL Multiphysics Reference Manual* see Table 2-4 for links to common sections and Table 2-5 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

	• Domain, Boundary, Edge, Point, and Pair Nodes for the Slip Flow Interface • Theory for the Slip Flow Interface In the *COMSOL Multiphysics Reference Manual:* • Pseudo Time Stepping for Laminar Flow Models • Handling Frames in Heat Transfer

	Slip Flow Benchmark: Application Library path **Microfluidics_Module/Rarefied_Flow/slip_flow_benchmark**

Domain, Boundary, Edge, Point, and Pair Nodes for the Slip Flow Interface

The Slip Flow Interface has these domain, boundary, edge, point, and pair nodes available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

	In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

	For axisymmetric components, COMSOL Multiphysics takes the axial symmetry boundaries (at $r = 0$) into account and automatically adds an **Axial Symmetry** node to the component that is valid on boundaries that represent the symmetry axis.

These nodes are available and described in this section (listed in alphabetical order):

- Continuity
- External Slip Wall
- Fluid
- Initial Values
- Interior Slip Wall
- Periodic Condition
- Slip Wall
- Symmetry

HEAT TRANSFER IN FLUIDS SUBMENU

These nodes and one subnode are described for the Heat Transfer interface in the *COMSOL Multiphysics Reference Manual* (listed in alphabetical order):

- Boundary Heat Source
- Heat Flux
- Heat Source
- Solid
- Line Heat Source
- Outflow
- Thickness
- Point Heat Source
- Heat Flux
- Temperature
- Thermal Insulation
- Thin Layer
- Translational Motion

LAMINAR FLOW SUBMENU

These nodes are described for the Laminar Flow interface in this guide (listed in alphabetical order):

- Boundary Stress
- Inlet
- Line Mass Source
- Open Boundary
- Outlet
- Point Mass Source
- Pressure Point Constraint
- Volume Force
- Wall

!	In the *COMSOL Multiphysics Reference Manual* see Table 2-4 for links to common sections and Table 2-5 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Fluid

The **Fluid** node prescribes its domains to be a fluid by adding momentum and energy transport equations.

HEAT CONDUCTION, FLUID

The default uses the **Thermal conductivity** k (SI unit: W/(m·K)) **From material**. For **User defined**, select **Isotropic**, **Diagonal**, **Symmetric**, or **Anisotropic** based on the characteristics of the thermal conductivity and enter another value or expression in the field or matrix.

	The thermal conductivity describes the relationship between the heat flux vector $\mathbf{q}$ and the temperature gradient ∇T as in $\mathbf{q} = -k\nabla T$ which is Fourier's law of heat conduction. Enter this quantity as power per length and temperature.

THERMODYNAMICS, FLUID

The **Fluid type** defaults to **Gas/Liquid**.

By default the **Density** ρ (SI unit: kg/m^3), **Heat capacity at constant pressure** C_p (SI unit: J/(kg·K)), and **Ratio of specific heats** γ(dimensionless) take values **From material**. For **User defined** to enter other values or expressions.

DYNAMIC VISCOSITY

The default **Dynamic viscosity** μ (SI unit: Pa·s) is taken **From material** or select **User defined**.

External Slip Wall

Use the **External Slip Wall** node to specify a wall with slip when the adjacent wall is external to the whole geometry. The wall temperature, wall velocity, and slip coefficients are specified. Constraint settings are specified, too.

SLIP WALL

Enter the components for the **Velocity of moving wall** $\mathbf{u}_\mathbf{w}$.

Enter a value or expression for the **Wall temperature** T_w. The default is 293.15 K.

Select the **Slip coefficients**: **Maxwell's model** (the default) or **User defined**.

Maxwell's Model

For **Maxwell's Model** enter values or expressions for the **Tangential momentum accommodation coefficient** α_v. The tangential accommodation coefficients are typically in the range of 0.85 to 1.0 and can be found in Ref. 4.

User defined

For **User defined** select a **Mean free path definition** — **Standard** (the default) or **Alternative (Sharipov)**. Then enter values for the following. Note that the defaults are different based on the Mean free path definition chosen.

- **Thermal slip coefficient** σ_T. The defaults are 1.2 for **Standard** and 1.1 for **Alternative (Sharipov)**.
- **Viscous slip coefficient** σ_S. The defaults are 1.1 for **Standard** and 1 for **Alternative (Sharipov)**.
- **Temperature jump coefficient** ζ_T. The defaults are 2.2 for **Standard** and 1.95 for **Alternative (Sharipov)**.

	Theoretical and experimental values of these coefficients for various gas surface combinations are available in Ref. 5. Note that it is more convenient to use the **Alternative (Sharipov)** mean free path definition when using this data.

CONSTRAINT SETTINGS

Choose between **Weak constraints** (default) and **Nitsche constraints**.

Initial Values

The **Initial Values** node adds initial values for the velocity field, pressure, and temperature. For the transient solver, these values define the state of the problem at the initial time step; for the stationary solver, they serve as a starting point for the nonlinear solver.

INITIAL VALUES

Enter values or expressions for the initial estimate the solver uses for the **Velocity field** $\mathbf{u}$, **Pressure** p, and **Temperature** T.

Slip Wall

Use the **Slip Wall** node to specify a wall with slip adjacent to a solid region in which the heat transfer equations are solved. A wall velocity can be specified along with the slip coefficients. Constraint settings are specified, too.

SLIP WALL

Enter the components for the **Velocity of moving wall** $\mathbf{u}_\mathbf{w}$. Select the **Slip coefficients**: **Maxwell's model** (the default) or **User defined**. These settings are the same as for External Slip Wall.

CONSTRAINT SETTINGS

Choose between **Weak constraints** (default) and **Nitsche constraints**.

Periodic Condition

The **Periodic Condition** node applies periodic boundary conditions for the fluid flow and the heat transfer equations, as appropriate.

For more information, see Periodic Boundary Conditions in the *COMSOL Multiphysics Reference Manual*.

CONSTRAINT SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options**.

Symmetry

The **Symmetry** node applies symmetry conditions for the fluid flow and heat transfer equations, as appropriate.

CONSTRAINT SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options**.

Interior Slip Wall

Use the **Interior Slip Wall** adds a wall with slip on interior boundaries. It is similar to the External Slip Wall boundary condition available on exterior boundaries except that it applies on both sides of an interior boundary. It allows discontinuities of the dependent variables across the boundary. Constraint settings are specified, too.

SLIP WALL

Enter the components for the **Velocity of moving wall** $\mathbf{u}_\mathbf{w}$.

Enter a value or expression for the **Wall temperature** T_w. The default is 293.15 K.

Select the **Slip coefficients**: **Maxwell's model** (the default) or **User defined**.

Maxwell's Model

For **Maxwell's Model** enter values or expressions for the **Tangential momentum accommodation coefficient** a_v. The tangential accommodation coefficients are typically in the range of 0.85 to 1.0 and can be found in Ref. 4.

User defined

For **User defined** select a **Mean free path definition** — **Standard** (the default) or **Alternative (Sharipov)**. Then enter values for the following. Note that the defaults are different based on the Mean free path definition chosen.

- **Thermal slip coefficient** σ_T. The defaults are 1.2 for **Standard** and 1.1 for **Alternative (Sharipov)**.
- **Viscous slip coefficient** σ_S. The defaults are 1.1 for **Standard** and 1 for **Alternative (Sharipov)**.
- **Temperature jump coefficient** ζ_T. The defaults are 2.2 for **Standard** and 1.95 for **Alternative (Sharipov)**.

	Theoretical and experimental values of these coefficients for various gas surface combinations are available in Ref. 5. Note that it is more convenient to use the **Alternative (Sharipov)** mean free path definition when using this data.

CONSTRAINT SETTINGS

Choose between **Weak constraints** (default) and **Nitsche constraints**.

Continuity

The **Continuity** node can be added to pairs. It prescribes that the temperature field is continuous across the pair. Continuity is only suitable for pairs where the boundaries match.

Since it is not usual to use an assembly to represent the fluid flow domains, **Continuity** is only appropriate between two domains in which **Heat Transfer in Solids** applies.

CONSTRAINT SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options**.

Theory for the Slip Flow Interface

The Slip Flow Interface theory is described in this section:

- Slip Flow Boundary Conditions
- References for the Slip Flow Interface

	If you have the Heat Transfer Module, the **Thin Layer** node (and subnodes) is also available. The feature and the background theory is described in the *Heat Transfer Module User's Guide*.

Slip Flow Boundary Conditions

Maxwell was the first person to consider the boundary conditions required for the solution of the Boltzmann equation in the case of a slightly rarefied gas (Ref. 1). The boundary conditions he derived can be used as boundary conditions for the Navier–Stokes equations in the slip-flow regime, although Maxwell considered the particular case of a monatomic hard-sphere gas, so some generalization is required.

Maxwell's boundary condition takes the form:

$$\mathbf{u}_{\text{slip}} = \frac{G}{\mu}(\tau\mathbf{n} - ((\mathbf{n}^T\tau\,\mathbf{n})\mathbf{n})) + \frac{3}{4}\frac{\mu}{\rho T_g}[\nabla\ - \mathbf{n}(\mathbf{n}\cdot\nabla\ )]\left[T_g - \frac{8}{3}G(\mathbf{n}\cdot\nabla T_g)\right] \quad (7\text{-}1)$$

where $\mathbf{u}_{\text{slip}}$ is the slip velocity, $\mathbf{n}$ is the boundary normal, τ is the viscous stress tensor, μ is the viscosity of the gas, ρ is its density, and T_g is its temperature. The factor G (which has dimensions of length) is given by:

$$G = \frac{2 - a_v}{a_v}\lambda$$

where λ is the mean free path and a_v is the tangential momentum accommodation coefficient (for a model in which the surface reflects some molecules diffusely and

some specularly, this is equivalent to the fraction of molecules which are reflected diffusely).

	A slightly different definition of the *mean free path* is used here: in terms of Maxwell's original parameter, l, the mean free path is $\lambda = 2l/3$. In Maxwell's original paper, he uses a coordinate based notation, the vector notation is available in Ref. 2.

In Equation 7-1 the left-hand term represents the phenomena of viscous slip, whilst the right-hand term produces thermal slip or transpiration. Maxwell was aware that the temperature of the gas was not necessarily equal to that of the wall but formulated the boundary condition using only the gas temperatures. When the wall temperature is included, the following equations are obtained (Ref. 2 and Ref. 3):

$$\mathbf{u}_{\text{slip}} = \sigma_s \frac{\lambda}{\mu}(\tau\mathbf{n} - ((\mathbf{n}^T \tau\, \mathbf{n})\mathbf{n})) + \sigma_T \frac{\mu}{\rho T_g}[\nabla T_w - (\mathbf{n} \cdot \nabla T_w)\mathbf{n}]$$
$$T_w = T_g - \zeta_T \lambda \mathbf{n} \cdot \nabla T_g$$

where T_w is the wall temperature, σ_s is the viscous slip coefficient, σ_T is the thermal slip coefficient, and ζ_T is the temperature jump coefficient. Within a generalized Maxwell's model the three coefficients σ_s, σ_T, and ζ_T are given by:

$$\sigma_s = \frac{2 - a_v}{a_v}$$
$$\sigma_T = \frac{3}{4} \tag{7-2}$$
$$\zeta_T = \frac{2 - a_v}{a_v} \frac{2\gamma}{\gamma + 1} \frac{\kappa}{\mu C_p}$$

where κ is the thermal conductivity of the gas. The mean free path can be computed from the gas properties using the following equation (Ref. 3):

$$\lambda = \frac{2\mu}{\rho \langle c \rangle}$$
$$\langle c \rangle = \left(\frac{8RT}{\pi M_n}\right)^{1/2} = \left(\frac{8p}{\pi\rho}\right)^{1/2} \tag{7-3}$$

consequently:

$$\lambda = \sqrt{\frac{\pi}{2\rho p}}\mu$$

In some cases an alternative definition of the mean free path, λ', is used (as, for example, in Ref. 5):

$$\lambda' = \frac{2}{\sqrt{\pi}}\lambda$$

It is possible to use this definition of the mean free path when entering user-defined values for the slip coefficients.

	Values of the parameters given in Equation 7-2, are available in Ref. 5, although care should be taken with the slip and temperature jump coefficients to adjust for differences between the author's definition of the mean free path and that used in COMSOL Multiphysics. Also note that the formulation assumes that the ideal gas laws apply. This assumption is implicit in the derivation of the above equations (Ref. 3) and at the level of approximation of the equations is reasonable.

	For mixtures of gases in which concentration gradients exist an additional term should be added to the slip on the wall. At present this feature is not implemented in COMSOL.

References for the Slip Flow Interface

1. J.C. Maxwell, "On Stresses in Rarefied Gases Arising from Inequalities of Temperature", *Phil. Trans. R. Soc. Lond.*, vol. 170, pp. 231–256, 1879.

2. D.A. Lockerby, J. M. Reese, D.R. Emerson, and R.W. Barber, "Velocity Boundary Condition at Solid Walls in Rarefied Gas Calculations", *Phys. Rev. E*, vol. 70, 017303, 2004.

3. E.H. Kennard, *Kinetic Theory of Gases*, McGraw Hill, New York, 1938.

4. G. Kariadakis, A. Beskok, and N. Aluru, *Microflows and Nanoflows*, Springer Science and Business Media, 2005.

5. F. Sharipov, "Data on the Velocity Slip and Temperature Jump on a Gas-Solid Interface", *J. Phys. Chem. Ref. Data*, vol. 40, no. 2, 023101, 2011.

8

Chemical Species Transport Interfaces

The Microfluidics Module has an enhanced version of the Transport of Diluted Species interface that is available with the basic COMSOL Multiphysics® license. In addition, the Transport of Diluted Species in Porous Media interface is available. Both physics interfaces are found under the **Chemical Species Transport** branch ( ).

In this chapter:

- The Transport of Diluted Species Interface
- The Transport of Diluted Species in Porous Media Interface
- Theory for the Transport of Diluted Species Interface

The Transport of Diluted Species Interface

The **Transport of Diluted Species (tds)** interface ( ), found under the **Chemical Species Transport** branch ( ), is used to calculate the concentration field of a dilute solute in a solvent. Transport and reactions of the species dissolved in a gas, liquid, or solid can be handled with this interface. The driving forces for transport can be diffusion by Fick's law, convection when coupled to a flow field, and migration, when coupled to an electric field.

The interface supports simulation of transport by convection and diffusion in 1D, 2D, and 3D as well as for axisymmetric components in 1D and 2D. The dependent variable is the molar concentration, c. Modeling multiple species transport is possible, whereby the physics interface solves for the molar concentration, c_i, of each species i.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `tds`.

DOMAIN SELECTION

If any part of the model geometry should not partake in the mass transfer model, remove that part from the selection list.

OUT-OF-PLANE THICKNESS

For 2D components, the **Thickness** field (default value: 1 m) defines a parameter for the thickness of the geometry perpendicular to the two-dimensional cross-section. Both constant and varying thicknesses are supported. The value of this parameter is used, among other things, to automatically calculate molar flow rates from the total molar flux.

CROSS-SECTIONAL AREA

For 1D components, enter a **Cross-sectional area** A_c (SI unit: m^2) to define a parameter for the area of the geometry perpendicular to the 1D component. Both constant and varying areas are supported. The value of this parameter is used, among other things, to automatically calculate molar flow rates from the total molar flux. The default is 1 m^2.

TRANSPORT MECHANISMS

Mass transport due to diffusion is always included. Use the checkboxes available under **Additional transport mechanisms** to control other transport mechanisms.

Note: Some of the additional transport mechanisms listed below are only available in certain products. For details see https://www.comsol.com/products/specifications/.

- By default, the **Convection** checkbox is selected. Clear the checkbox to disable convective transport.
- Select the **Migration in electric field** checkbox to activate transport of ionic species in an electric field. See further the theory section Adding Transport Through Migration.

!	Transport of ionic species in an electric field is available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

Mass Transport in Porous Media

The **Mass transport in porous media** checkbox activates functionality specific to species transport in porous media:

- Porous Medium
- Unsaturated Porous Medium
- Porous Electrode Coupling

- Volatilization
- Species Source

!	Note: Mass transport in porous media is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

CONSISTENT STABILIZATION

To display this sections, click the **Show** button ( ) and select **Stabilization**.

- When the **Crosswind diffusion** checkbox is selected, a weak term that reduces spurious oscillations is added to the transport equation. The resulting equation system is always nonlinear. There are two options for the **Crosswind diffusion type**:
  - **Do Carmo and Galeão** — the default option. This type of crosswind diffusion reduces undershoots and overshoots to a minimum but can in rare cases give equation systems that are difficult to fully converge.
  - **Codina** — this option is less diffusive compared to the Do Carmo and Galeão option but can result in more undershoots and overshoots. It is also less effective for anisotropic meshes. The Codina option activates a text field for the **Lower gradient limit** g_{lim}. Its defaults to `0.1[mol/m^3]/tds.helem`, where `tds.helem` is the local element size.
- For both consistent stabilization methods, select an **Equation residual**. **Approximate residual** is the default and means that derivatives of the diffusion tensor components are neglected. This setting is usually accurate enough and is computationally faster. If required, select **Full residual** instead.

INCONSISTENT STABILIZATION

To display this section, click the **Show** button ( ) and select **Stabilization**. By default, the **Isotropic diffusion** checkbox is not selected, because this type of stabilization adds artificial diffusion and affects the accuracy of the original problem. However, this option can be used to get a good initial guess for under resolved problems.

ADVANCED SETTINGS

To display this section, click the **Show** button ( ) and select **Advanced Physics Options**. Normally these settings do not need to be changed. Select a **Material Balance Form** —

Nonconservative (the default) or **Conservative**. The conservative formulation should be used for compressible flow. See Material Balance Formulation for more information.

DISCRETIZATION

To display all settings available in this section, click the **Show** button (👁) and select **Advanced Physics Options**.

The **Compute boundary fluxes** checkbox is activated by default so that COMSOL Multiphysics computes predefined accurate boundary flux variables. When this option is selected, the solver computes variables storing accurate boundary fluxes from each boundary into the adjacent domain.

If the checkbox is cleared, the COMSOL Multiphysics software instead computes the flux variables from the dependent variables using extrapolation, which is less accurate in postprocessing results but does not create extra dependent variables on the boundaries for the fluxes.

The flux variables affected in the interface are:

- `ndflux_`*c* (where *c* is the dependent variable for the concentration). This is the normal diffusive flux and corresponds to the boundary flux when diffusion is the only contribution to the flux term.
- `ntflux_`*c* (where *c* is the dependent variable for the concentration). This is the normal total flux and corresponds to the boundary flux plus additional transport terms, for example, the convective flux when you use the nonconservative form.

Also the **Apply smoothing to boundary fluxes** checkbox is available if the previous checkbox is selected. The smoothing can provide a more well-behaved flux value close to singularities.

For details about the boundary fluxes settings, see Computing Accurate Fluxes in the *COMSOL Multiphysics Reference Manual*.

The **Value type when using splitting of complex variables** setting should in most pure mass transfer problems be set to **Real**, which is the default. It makes sure that the dependent variable does not get affected by small imaginary contributions, which can occur, for example, when combining a Time Dependent or Stationary study with a frequency-domain study. For more information, see Splitting Complex-Valued Variables in the *COMSOL Multiphysics Reference Manual*.

DEPENDENT VARIABLES

The dependent variable name is the **Concentration** *c* by default. The names must be unique with respect to all other dependent variables in the component.

Add or remove species variables in the model and also change the names of the dependent variables that represent the species concentrations.

Enter the **Number of species**. Use the **Add concentration** (+) and **Remove concentration** ( ) buttons as needed.

FURTHER READING

	• Theory for the Transport of Diluted Species Interface • Numerical Stabilization in the *COMSOL Multiphysics Reference Manual*. • In the *COMSOL Multiphysics Reference Manual*, see Table 2-4 for links to common sections and Table 2-5 for common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

	• *Effective Diffusivity in Porous Materials*: Application Library path **COMSOL_Multiphysics/Diffusion/effective_diffusivity** • *Micromixer*: Application Library path **COMSOL_Multiphysics/Fluid_Dynamics/micromixer**

The Transport of Diluted Species in Porous Media Interface

This interface ( ), found under the **Chemical Species Transport** branch ( ), is used to calculate the species concentration and transport in free and porous media. The interface is the same as the *Transport of Diluted Species* interface but it uses other defaults: The Mass Transport in Porous Media property is selected, and a Porous Medium node is added by default. The interface includes reaction rate expressions and solute sources for modeling of species transport and reaction in porous media.

This interface is dedicated to modeling transport in porous media, including immobile and mobile phases, where the chemical species may be subjected to diffusion, convection, migration, dispersion, adsorption, and volatilization in porous media. It

supports cases where either the solid phase substrate is exclusively immobile, or when a gas-filling medium is also assumed to be immobile.

It applies to one or more diluted species or solutes that move primarily within a fluid that fills (saturated) or partially fills (unsaturated) the voids in a solid porous medium. The pore space not filled with fluid contains an immobile gas phase. Models including a combination of porous media types can be studied.

The main feature nodes are the **Porous Medium** and **Unsaturated Porous Medium** nodes, which add the equations for the species concentrations and provide an interface for defining the properties of the porous media, as well as additional properties governing adsorption, volatilization, dispersion and diffusion, migration, and the velocity field to model convection.

The physics interface can be used for stationary and time-dependent analysis.

When this physics interface is added, these default nodes are also added to the **Model Builder** — **Porous Medium**, **No Flux** (the default boundary condition), and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions, reaction rate expressions, and species sources. You can also right-click **Transport of Diluted Species in Porous Media** to select physics features from the context menu.

SETTINGS

The rest of the settings are the same as The Transport of Diluted Species Interface.

FURTHER READING

	• Mass Balance Equation for Transport of Diluted Species in Porous Media • Domain, Boundary, and Pair Nodes for the Transport of Diluted Species Interface

	• *Variably Saturated Flow and Transport — Sorbing Solute*: Application Library path **Subsurface_Flow_Module/Solute_Transport/sorbing_solute** Web link: https://www.comsol.com/model/variably-saturated-flow-and-transport-sorbing-solute-490

Domain, Boundary, and Pair Nodes for the Transport of Diluted Species Interface

The Transport of Diluted Species Interface has the following domain, boundary, point, and pair nodes, listed in alphabetical order, available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or by right-clicking to access the context menu (all users).

- To add a node, go to the **Physics** toolbar, no matter what operating system you are using.
- Contextual subnodes (attributes) are available by clicking the parent node in the Model Builder, and then selecting the subnode from the **Attributes** menu.

- Adsorption
- Concentration
- Continuity on Interior Boundaries
- Dispersion
- Electrode Surface Coupling
- Equilibrium Reaction
- Fast Irreversible Surface Reaction
- Fluid
- Fluid (Porous Medium)
- Flux
- Flux Discontinuity
- Fracture
- Gas
- Inflow
- Initial Values
- Line Mass Source
- Liquid
- Mass-Based Concentrations
- No Flux
- Open Boundary
- Out-of-Plane Flux
- Outflow
- Partition Condition
- Periodic Condition
- Point Mass Source
- Porous Matrix
- Porous Medium
- Porous Electrode Coupling
- Reaction Coefficients
- Reactions
- Solid
- Species Properties
- Species Source
- Surface Reactions
- Surface Equilibrium Reaction
- Symmetry
- Thin Diffusion Barrier
- Thin Impermeable Barrier
- Unsaturated Porous Medium
- Volatilization

Some features require certain add-on modules. For details see https://www.comsol.com/products/specifications/

For axisymmetric components, COMSOL Multiphysics takes the axial symmetry boundaries (at $r = 0$) into account and automatically adds an **Axial Symmetry** node that is valid on boundaries representing the symmetry axis.

!	In the *COMSOL Multiphysics Reference Manual*, see Table 2-4 for links to common sections and Table 2-5 for common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Prescribing Conditions on Fluid-Solid Interfaces

Defining conditions on interfaces between different phases, typically a wall in contact with a fluid, it is worthwhile to be careful with how variables in the conditions are evaluated. COMSOL Multiphysics supports that variables are defined differently on adjacent domains (or any other geometry dimension). Evaluating a variable with differing definitions, the mean value is returned on a boundary separating the different domains. The density, pressure, or temperature are examples of variables that may differ in a fluid and a solid. In order to specify on which side a variable is evaluated, the up and down operators (described in the *COMSOL Multiphysics Reference Manual*) can be used.

Species Properties

Use this node to define parameters specific to each of the species. It is available when the **Migration in electric field** checkbox is selected in the Transport Mechanisms section of the interface.

The node will change its label depending on what inputs are available in the node. If only **Charge** is available, it will be labeled "Species charges".

CHARGE

Enter the charge number z_c (dimensionless, but requires a plus or minus sign) for each species.

ACTIVITY

This section is available when the **Species Activity** combo box is set to **Debye–Hückel** or **User defined**.

If **Debye–Hückel** is selected, enter the ion size number, a_0, for each species. If **User defined** is selected, enter the activity coefficient, f, for each species.

Fluid

The settings in this node are dependent on the checkboxes selected under Transport Mechanisms in the **Settings** window for the Transport of Diluted Species interface. It includes only the sections required by the activated transport mechanisms. It has all the equations defining transport of diluted species as well as inputs for the material properties.

MODEL INPUTS

The temperature model input is always available. Select the source of the **Temperature**. For **User defined**, enter a value or expression for the temperature in the input field. This input option is always available.

You can also select the temperature solved for by a Heat Transfer interface added to the model component. These physics interfaces are available for selection in the **Temperature** list.

CONVECTION

If transport by convection is active, the velocity field of the solvent needs to be specified. Select the source of the **Velocity field**. For **User defined**, enter values or expressions for the velocity components in the input fields. This input option is always available.

You can also select the velocity field solved for by a Fluid Flow interface added to the model component. These physics interfaces are available for selection in the **Velocity field** list.

DIFFUSION

Use this section to specify diffusion coefficients describing the diffusion of each species in the solvent fluid.

Use the **Source** list to select diffusion coefficients defined in a material or a Chemistry interface.

Select **Material** to use a diffusion coefficient in a material available in the model. User-defined property groups including a diffusion coefficient output property are available for selection in the **Fluid diffusion coefficient** list.

Select **Chemistry** to use a diffusion coefficient from a Chemistry interface added to model component. Diffusion coefficients are automatically defined when **Calculate transport properties** is selected on the interface level of a Chemistry interface. All

defined diffusion coefficients are available for selection in the **Fluid diffusion coefficient** list.

For **User defined**, enter a value or expression for the **Fluid diffusion coefficient** D_c of each species in the corresponding input field. This can be a scalar value for isotropic diffusion or a tensor describing anisotropic diffusion. Select the appropriate tensor type — **Isotropic**, **Diagonal**, **Symmetric**, or **Full** that describes the diffusion transport, and then enter the values in the corresponding element (one value for each species).

Note that multiple species, as well as Migration in Electric fields (described below) is only available for certain COMSOL Multiphysics add-on products. See details: https://www.comsol.com/products/specifications/.

MIGRATION IN ELECTRIC FIELD

This section is available when the **Migration in electric field** checkbox is selected. From the **Electric potential** list, select the source of the electric field.

- Enter a value or expression for the **Electric potential** V, which is **User defined**; this input option is always available.
- Select the electric potential solved by an AC/DC-based interface that has also been added to the model.
- Select the electric potential defined or solved by Electrochemistry interface that has been added to the component.

By default the **Mobility** is set to be calculated based on the species diffusivity and the temperature using the **Nernst-Einstein relation**. For **User defined**, and under **Mobility**, select the appropriate scalar or tensor type — **Isotropic**, **Diagonal**, **Symmetric**, or **Full** — and type in the value of expression of the mobility $u_{m,c}$.

Enter the **Charge number** z_c (dimensionless, but requires a plus or minus sign) for each species.

The temperature (if you are using mobilities based on the Nernst–Einstein relation) is taken from **Model Inputs** section.

Note that the migration in electric fields feature is only available in some COMSOL products. See details: https://www.comsol.com/products/specifications/.

EXAMPLE MODELS

	• *Separation Through Dialysis*: Application Library path **Chemical_Reaction_Engineering_Module/Mixing_and_Separation/dialysis** Web link: https://www.comsol.com/model/separation-through-dialysis-258

	• *Transport in an Electrokinetic Valve*: Application Library path **Microfluidics_Module/Fluid_Flow/electrokinetic_valve** Web link: https://www.comsol.com/model/transport-in-an-electrokinetic-valve-603

Solid

Use this node to describe diffusion in a solid phase domain. In this feature, the activities of the species are assumed to be ideal.

DIFFUSION

Specify the diffusion coefficients describing the diffusion of each species in the solid.

Enter a value or expression for the **Diffusion coefficient** D_c of each species in the corresponding input field. This can be a scalar value for isotropic diffusion or a tensor describing anisotropic diffusion. Select the appropriate tensor type — **Isotropic**, **Diagonal**, or **Symmetric** that describes the diffusion transport, and then enter the values in the corresponding element (one value for each species).

ADVANCED

This section is only available with the **Advanced Physics Options** selected and when the model contains a split between the material frame and the spatial frame. A split of these frames occurs when using a **Moving Mesh** node or a Structural Mechanics interface like **Solid Mechanics**. In such a model, the reference geometry (the material frame) differs from the deformed geometry (the spatial frame). The diffusive transport of species is solved for on the material frame, but the equation is adjusted for geometry deformations so that species conservation is achieved on the spatial frame. Use the **Diffusion model** to define the frame of reference for the diffusion tensor.

Select **Reference geometry based (Lagrangian)** to specify the diffusion tensor in the undeformed geometry, implying that the diffusion is defined in the material frame (indicated by coordinates X, Y, Z). This is the preferred setting for an anisotropic diffusion in combination with solid body translation or rotation. Also in general when the diffusion tensor components have been measured in an undeformed geometry.

Select **Deformed geometry based (Eulerian)** to specify the diffusion tensor in the deformed geometry. This means that the diffusion is defined in the spatial frame (indicated by coordinates x, y, z). Use this setting when the diffusion tensor components have been measured in a deformed geometry.

The **Advanced Physics Options** is found in the **Show More Options** dialog, accessed by clicking the **Show More Options** button ( ).

Note that multiple species are only available for certain COMSOL Multiphysics add-on products. See details: https://www.comsol.com/products/specifications/.

Initial Values

The **Initial Values** node specifies the initial values for the concentration of each species. These serve as an initial guess for a stationary solver or as initial conditions for a transient simulation.

DOMAIN SELECTION

If there are several types of domains with different initial values defined, it might be necessary to remove some domains from the selection. These are then defined in an additional **Initial Values** node.

INITIAL VALUES

Enter a value or expression for the initial value of the **Concentration** or concentrations, c_i. This also serves as a starting guess for stationary problems.

Mass-Based Concentrations

Use the **Mass-Based Concentrations** node to add postprocessing variables for mass-based concentrations (SI unit: $\mathrm{kg/m^3}$) and mass fractions (dimensionless) for all species.

MIXTURE PROPERTIES

The default **Solvent density** ρ_{solvent} is taken **From material**. For **User defined**, enter a value or expression manually. Define the **Molar mass** of each species, which is needed to calculate the mass-based concentration.

Reactions

Use the **Reactions** node to account for the consumption or production of species through chemical reactions. Define the rate expressions as required.

DOMAIN SELECTION

From the **Selection** list, choose the domains on which to define rate expression or expressions that govern the source term in the transport equations.

Several reaction nodes can be used to account for different reactions in different parts for the modeling geometry.

REACTION RATES

Add a rate expression R_i (SI unit: mol/(m^3·s)) for species i. Enter a value or expression in the field. Note that if you have the *Chemistry* interface available, provided with the *Chemical Reaction Engineering Module*, the reaction rate expressions can be automatically generated and picked up using the drop-down lists. For an example, see the application *Fine Chemical Production in a Plate Reactor* as linked below.

REACTING VOLUME

This section is only available when the Mass Transport in Porous Media property is available and selected. See https://www.comsol.com/products/specifications/ for more details on availability.

When specifying reaction rates for a species in porous media, the specified reaction rate may have the basis of the total volume, the pore volume, or in the case of using the volume of a particular phase (applicable when modeling an unsaturated porous medium).

- For **Total volume**, the reaction expressions, in mol/(m^3·s), are specified per unit volume of the model domain (multiplied by unity).
- For **Pore volume**, the reaction expressions, in mol/(m^3·s), are specified per unit volume of total pore space. The reaction expressions will be multiplied by the domain porosity, ε_p. (ε_p equals unity for nonporous domains).

- For **Liquid phase**, the reaction expressions, in mol/(m^3·s), are specified per unit volume of liquid in the pore space. The expressions will be multiplied by the liquid volume fraction θ_l. (θ_l equals the porosity (ε_p) on Porous Medium domains).
- For **Gas phase**, the reaction expressions, in mol/(m^3·s), are multiplied by the gas volume fraction $\theta_g = \varepsilon_p - \theta_l$. θ_g equals 0 for Porous Medium domains.

FURTHER READING

See the theory chapter on chemical species transport, starting with the section *Mass Balance Equation*.

	• *Fine Chemical Production in a Plate Reactor*: Application Library path **Chemical_Reaction_Engineering_Module/Reactors_with_Mass_and_Heat_Transfer/plate_reactor** Web link: https://www.comsol.com/model/fine-chemical-production-in-a-plate-reactor-8589

No Flux

This node is the default boundary condition on exterior boundaries. It should be used on boundaries across which there is no mass flux, typically solid walls where no surface reactions occur. The condition applied for each species corresponds to

$$-\mathbf{n} \cdot (-D\nabla c) = 0$$

where $\mathbf{n}$ denotes the outward pointing normal of the boundary. When the mass transport includes migration of ionic species, the no flux condition is:

$$-\mathbf{n} \cdot (-D\nabla c - zu_m Fc\nabla\phi) = 0$$

CONVECTION

By default, the feature prescribes a vanishing flux due to diffusion and migration in an electric field. This is the appropriate no flux condition when the relative convective velocity at the boundary is zero. When the fluid velocity at the boundary is not equal to that of the boundary, it is often convenient to prescribe the total flux including the convection. To do this select **Include** in the **Convection** section.

When including the convection, the no flux condition prescribed is

$$-\mathbf{n}\cdot(-D\nabla c+\mathbf{u}c) = 0$$

or

$$-\mathbf{n}\cdot(-D\nabla c-zu_{\mathrm{m}}Fc\nabla\phi+\mathbf{u}c) = 0$$

when migration of ionic species is included.

Inflow

Use this node to specify all species concentrations at an inlet boundary.

If you want to specify the concentration of a subset of the partaking species, this can be done by using the Concentration node instead.

For the **Electroanalysis** interface, this node is available when you select the **Convection** checkbox on the physics interface **Settings** window.

CONCENTRATION

For the concentration of each species $c_{0,c}$ (SI unit: mol/m^3), enter a value or expression.

BOUNDARY CONDITION TYPE

The option **Concentration constraint** constrains the concentration values on the boundary by the use of pointwise constraints.

The other option, **Flux (Danckwerts)** can be used when the concentration at the boundary is not known, or when it varies in a nontrivial manner. This may, for example, be useful when reactions with high reaction rates occur in the vicinity of the inlet. In this case the concentration far upstream of the boundary is instead prescribed. The **Flux (Danckwerts)** condition prescribes the total flux defined by the upstream concentration and the fluid velocity at the boundary.

CONSTRAINT SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options**. You can find details about the different constraint settings in the section Constraint Reaction Terms in the *COMSOL Multiphysics Reference Manual*.

FURTHER READING

See the theory chapter in the section Danckwerts Inflow Boundary Condition.

Outflow

Apply this condition at outlets boundaries where species should be transported out of the model domain by fluid motion or by an electric field (in the case of ions). It is assumed that convection and migration (in an electric field) are the dominating transport mechanisms across the boundary, and therefore that the diffusive transport can be ignored, that is:

$$\mathbf{n} \cdot (-D\nabla c) = 0$$

Note that the **Convection** or the **Migration in electric field** transport mechanisms needs to be included for this node to be available.

Concentration

This condition node adds a boundary condition for the species concentration. For example, a $c = c_0$ condition specifies the concentration of species c.

CONCENTRATION

Individually specify the concentration for each species. Select the checkbox for the **Species** to specify the concentration, and then enter a value or expression in the corresponding field. To use another boundary condition for a specific species, click to clear the checkbox for the concentration of that species.

When defining conditions on boundaries between different phases, see the section Prescribing Conditions on Fluid-Solid Interfaces.

CONSTRAINT SETTINGS

To display this section, click the **Show** button ( ) and select **Advanced Physics Options**. You can find details about the different constraint settings in the section Constraint Reaction Terms in the *COMSOL Multiphysics Reference Manual*.

Flux

This node can be used to specify the species molar flux across a boundary. The flux can for example occur due to chemical reactions or a phase change at the boundary. The flux can also represent the transport to or from a surrounding environment currently not included model.

The prescribed flux of a species c is by default defined as

$$-\mathbf{n} \cdot (-D\nabla c) = J_0$$

where **n** denotes the outward pointing normal of the boundary. When the mass transport includes migration of ionic species, the flux is defined as:

$$-\mathbf{n} \cdot (-D\nabla c - zu_{\mathrm{m}}Fc\nabla\phi) = J_0$$

The flux prescribed, J_0, can include any arbitrary user-specified expression. It can be constant or a function of a dependent variable or independent variable. Common examples are a flux dependent of the concentration, temperature, pressure, or the electric potential ϕ.

When defining conditions on boundaries between different phases, see the section Prescribing Conditions on Fluid-Solid Interfaces.

CONVECTION

By default, the flux due to diffusion and migration in an electric field is prescribed. This is the appropriate flux condition when the relative velocity at the boundary is zero. When the fluid velocity is not equal to that of the boundary, it is often convenient to prescribe the total flux, including the convection. To do this select **Include** in the **Convection** section.

When including the convection, the prescribed flux is defined as:

$$-\mathbf{n} \cdot (-D\nabla c + \mathbf{u}c) = J_0$$

or

$$-\mathbf{n} \cdot (-D\nabla c - zu_{\mathrm{m}}Fc\nabla\phi + \mathbf{u}c) = J_0$$

when migration of ionic species is included.

INWARD FLUX

Select the Species checkbox for the species for which to specify the flux, and enter a value or expression for the inward flux in the corresponding field. Use a minus sign when specifying a flux directed out of the system. To use another boundary condition for a specific species, click to clear the checkbox for that species.

External convection

Set **Flux type** to **External convection** to prescribe a flux to or from an exterior domain (not modeled) assumed to include convection. The exterior can for example include a

forced convection to control the temperature or to increase the mass transport. In this case the prescribed mass flux corresponds to

$$J_0 = k_c(c_b - c)$$

where k_c is a mass transfer coefficient and c_b is the bulk concentration, the typical concentration far into the surrounding exterior domain.

Symmetry

The **Symmetry** node can be used to represent boundaries where the species concentration is symmetric, that is, where there is no mass flux across the boundary.

This boundary condition is identical to that of the No Flux node.

Flux Discontinuity

This node represents a discontinuity in the mass flux across an interior boundary:

$$-\mathbf{n} \cdot [(\mathbf{J} + \mathbf{u}c)_u - (\mathbf{J} + \mathbf{u}c)_d] = N_0 \qquad \mathbf{J} = -D\nabla c - zu_m Fc\nabla\phi$$

where the value N_0 (SI unit: mol/(m^2·s)) specifies the jump in total flux at the boundary. This can be used to model a boundary source, for example a surface reaction, adsorption, or desorption.

FLUX DISCONTINUITY

In this section the jump in species flux (or surface source) is specified.

Select the Species checkbox for the species to specify and enter a value or expression for the material flux jump in the corresponding field. To use a different boundary condition for a specific species, click to clear the checkbox for the flux discontinuity of that species.

Partition Condition

The **Partition Condition** node can be used to prescribe the relation between the concentration of a solute species in two adjoining immiscible phases. It can for example be used on interior boundaries separating two liquid phases, a gas-liquid interface, or on a boundary separating a liquid phase and a solid or porous media.

Select **Partition coefficient** from the **Relation** list to prescribe a linear relationship between the concentration on either side of a boundary. For a species concentration

c_i, the ratio between the concentration on the upside and on the downside of the boundary ($c_{i,\mathrm{u}}$ and $c_{i,\mathrm{d}}$ respectively) is then defined in terms of a partition coefficient K_i in the manner of

$$K_i = \frac{c_{i,\,\mathrm{u}}}{c_{i,\,\mathrm{d}}}$$

Use the associated input field to prescribe the partition coefficient for each species.

Select **User defined** from the **Relation** list to set up a nonlinear relation between the up and downside concentrations. For such relations $f(c_i)_\mathrm{u} = f(c_i)_\mathrm{d}$, where $f(c_i)_\mathrm{u}$ is the expression enforced on the upside. Use the associated input fields to enter the upside and downside expressions for each species.

The up and downside of the selected boundary is indicated with a red arrow in the Graphics window. The arrow points from the downside into the upside. Select the **Reverse direction** checkbox to reverse the direction of the arrow on the selected boundary, and update the definition of the up and downside concentrations accordingly.

!	This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

FURTHER READING

For an example of using a partition condition, see this application example:

	Separation Through Dialysis: Application Library path **Chemical_Reaction_Engineering_Module/Mixing_and_Separation/dialysis**

Periodic Condition

The **Periodic Condition** node can be used to define periodicity for the mass transport between two sets of boundaries. The node prescribes continuity in the concentration and the mass flux between the “source” and the “destination” side, respectively. Note that these names are arbitrary and does not influence the direction in which mass is transported. It is dictated by mass transfer equations in the adjacent domains.

BOUNDARY SELECTION

The node can be activated on more than two boundaries, in which case the feature tries to identify two separate surfaces that each consist of one or several connected boundaries.

DESTINATION SELECTION

For more complex geometries, it might be necessary to specify the destination selection manually. To do so, right-click the **Periodic Condition** node and choose **Manual Destination Selection**. You can then specify the boundaries that constitute the destination surfaces in the **Destination Selection** section.

CONSTRAINT SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog. This section contains settings for specifying the type of constraint and whether to use a pointwise or weak constraint. See Constraint Settings for more information.

ORIENTATION OF SOURCE

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog. For information about the **Orientation of Source** section, see Orientation of Source and Destination.

ORIENTATION OF DESTINATION

This section appears if the setting for **Transform to intermediate map** in the **Orientation of Source** section is changed from the default value, **Automatic**, and **Advanced Physics Options** is selected in the **Show More Options** dialog. For information about the **Orientation of Destination** section, see Orientation of Source and Destination.

MAPPING BETWEEN SOURCE AND DESTINATION

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog. For information about the **Mapping Between Source and Destination** section, see Mapping Between Source and Destination.

FURTHER READING

For an example of using a periodic condition, see this application example:

	The KdV Equation and Solitons: Application Library path **COMSOL_Multiphysics/Equation_Based/kdv_equation**

Line Mass Source

The **Line Mass Source** feature models mass flow originating from a tube or line region with an infinitely small radius.

!	This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

SELECTION

The **Line Mass Source** feature is available for all dimensions, but the applicable selection differs between the dimensions.

MODEL DIMENSION	APPLICABLE GEOMETRICAL ENTITY
2D	Points
2D Axisymmetry	Points not on the symmetry axis and the symmetry axis
3D	Edges

SPECIES SOURCE

Enter the source strength, $\dot{q}_{l,c}$, for each species (SI unit: mol/(m·s)). A positive value results in species injection from the line into the computational domain, and a negative value means that the species is removed from the computational domain.

Line sources located on a boundary affect the adjacent computational domains. This effect makes the physical strength of a line source located in a symmetry plane twice the given strength.

FURTHER READING

See the section Mass Sources for Species Transport.

Point Mass Source

The **Point Mass Source** feature models mass flow originating from an infinitely small domain around a point.

!	This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

SPECIES SOURCE

Enter the source strength, $\dot{q}_{p,c}$, for each species (SI unit: mol/s). A positive value results in species injection from the point into the computational domain, and a negative value means that the species is removed from the computational domain.

Point sources located on a boundary or on an edge affect the adjacent computational domains. This has the effect, for example, that the physical strength of a point source located in a symmetry plane is twice the given strength.

FURTHER READING

See the section Mass Sources for Species Transport.

Open Boundary

Use this node to set up mass transport across boundaries where both convective inflow and outflow can occur. On the parts of the boundary where fluid flows into the domain, an exterior species concentration is prescribed. On the remaining parts, where fluid flows out of the domain, a condition equivalent to the **Outflow** node is instead prescribed.

The direction of the flow across the boundary is typically calculated by a fluid flow interface and is provided as a model input to the Transport of Diluted Species interface.

!	This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

EXTERIOR CONCENTRATION

Enter a value or expression for the **Exterior concentration**.

Thin Diffusion Barrier

Use this boundary condition to model a thin layer through which mass is transported by diffusion only. The node is applicable on interior boundaries and can be used to avoid meshing thin structures.

THIN DIFFUSION BARRIER

Specify the **Layer thickness**, d_s, and input a **Diffusion coefficient**, $D_{s,c}$, for each of the species included.

Thin Impermeable Barrier

This feature models a thin mass transfer barrier. It is available on interior boundaries and introduces a discontinuity in the concentration across the boundary. On each side, a no-flux condition is prescribed for the mass transport implying that it acts as a barrier. The feature can be used to avoid meshing thin structures.

Solving a model involving coupled fluid flow and mass transfer, the Thin Impermeable Barrier feature can be combined with an Interior Wall feature in order to model a thin solid wall.

Equilibrium Reaction

Use this node to model a reaction where the kinetics is so fast that the equilibrium condition is fulfilled at all times. The node solves for an additional degree of freedom (the reaction rate R_{eq}) to fulfill the equilibrium condition at all times in all space coordinates.

If the **Apply equilibrium condition on inflow boundaries** checkbox is selected, the specified inflow concentration values in all active **Inflow** boundary nodes for the physics interface are modified to comply with the equilibrium condition.

!	• A necessary requirement for this is feature to be available is that two or more species are solved for by the interface. • This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

EQUILIBRIUM CONDITION

The list defaults to **Equilibrium constant** or select **User defined**. For either option, the **Apply equilibrium condition on inflow boundaries** checkbox is selected by default.

For **Equilibrium constant**, enter an **Equilibrium constant** K_{eq} (dimensionless). Also enter a value or expression for the **Unit activity concentration** C_{a0} (SI unit: mol/m^3).

Selecting **Equilibrium constant** defines an equilibrium condition based on the stoichiometric coefficients, the species activities, and the law of mass action.

For **User defined**, enter an **Equilibrium expression** E_{eq} (dimensionless).

STOICHIOMETRIC COEFFICIENTS

Enter a value for the stoichiometric coefficient ν_c (dimensionless). The default is 0. Use negative values for reactants and positive values for products in the modeled reaction.

Species with a stoichiometric coefficient value of 0 are not affected by the **Equilibrium Reaction** node.

Surface Reactions

The **Surface Reactions** node can be used to account for the species boundary flux due to chemical reactions occurring on a surface (heterogeneous reactions). For a domain species participating in a surface reaction, the boundary flux corresponds to the reaction rate at the surface.

SURFACE REACTION RATE

Specify the surface reaction rate J_0 of each species resulting from the reactions. Note that if you have the Chemistry interface available, provided with the Chemical Reaction Engineering Module, the reaction rate expressions can be automatically generated and picked up using the drop-down list.

When defining conditions on boundaries between different phases, see the section Prescribing Conditions on Fluid-Solid Interfaces.

FURTHER READING

For an example of using the Surface Reactions node, see this application example:

	Chemical Vapor Deposition of GaAs: Application Library path **Chemical_Reaction_Engineering_Module/Reactors_with_Mass_and_Heat_Transfer/gaas_cvd**

Surface Equilibrium Reaction

Use this node to model an equilibrium reaction on a boundary (surface). The settings for this node are similar to Equilibrium Reaction. Note that a necessary requirement

for this is feature to be available is that two or more species are solved for by the interface.

When defining conditions on boundaries between different phases, see the section Prescribing Conditions on Fluid-Solid Interfaces.

!	This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

Fast Irreversible Surface Reaction

This boundary node defines an irreversible reaction where the kinetics is so fast that the only factor limiting the reaction rate is the transport of a species to the reacting surface.

The node will set the **Rate limiting species concentration to zero** at the boundary, and balance the fluxes of the species participating in the reaction and the current densities according to the Stoichiometric Coefficients settings.

When defining conditions on boundaries between different phases, see the section Prescribing Conditions on Fluid-Solid Interfaces.

!	This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

Porous Electrode Coupling

Use this node to add a molar source in a domain that is coupled to one or multiple Porous Electrode Reaction nodes of an Electrochemistry Interface.

The molar source is calculated from the number of electrons, stoichiometric coefficients, and volumetric current densities of the coupled porous electrode reactions specified in the **Reaction Coefficients** subnodes.

In the Transport of Concentrated Species interface, the molar sources (or sinks) are multiplied by the species molar masses to obtain the corresponding mass sources.

Additional Reaction Coefficients subnodes are available from the context menu (right-click the parent node) as well as from the **Physics** toolbar, **Attributes** menu.

Note that if you are also modeling the momentum transport and expect a nonnegligible total mass source or sink, which is often the case in gas diffusion electrodes, you need to also add a corresponding mass source/sink in the Fluid Flow interface. (A **Reacting Flow** multiphysics node adds the associated source/sink term in a Fluid Flow interface automatically.)

!	This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

Reaction Coefficients

Add this node to the Electrode Surface Coupling and Porous Electrode Coupling features to define molar fluxes and sources based on electrode current densities in an **Electrochemistry** interface.

The molar flux or source is proportional to the stoichiometric coefficients and the current density according to Faraday's law.

Current densities from **Electrode Reaction** (i_{loc}, SI unit: $\mathrm{A/m^2}$) or **Porous Electrode Reaction** nodes (i_{v}, SI unit: $\mathrm{A/m^3}$) of any **Electrochemistry** interface in the model are available for selection as the **Coupled reaction**, and user-defined expressions are also supported.

Enter the **Number of participating electrons** n_m (dimensionless) and the **Stoichiometric coefficient** v_c (dimensionless) as explained in the theory section linked below.

Use multiple subnodes to couple to multiple reactions.

Electrode Surface Coupling

Use this node to define a flux boundary condition based on current densities of one or multiple Electrode Reaction nodes in an Electrochemistry interface.

The flux is proportional to the current densities and the stoichiometric coefficients according to Faraday's law as defined by summation over the Reaction Coefficients subnodes.

Note that if you are also modeling the momentum transport and expect a nonnegligible total mass flux over the boundary, which is often the case for gas diffusion electrodes, you need to also add a corresponding Electrode Surface Coupling node in the Fluid Flow interface.

!	This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

Porous Medium

Use this node to model the concentration of diluted species transported by a solvent (mobile fluid phase) through interstices in a solid porous medium. In addition to transport due to convection and diffusion, the node contains functionality to include species evolution through adsorption and dispersion.

!	This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

Species transport through a porous medium is affected both by properties of the fluid phase, and as well as properties of the solid matrix. These properties are defined in the Fluid (Porous Medium) and Porous Matrix subnodes respectively. The Porous Medium node supports material properties using a Porous Material node, where properties are defined per phase in a similar manner.

Add an Adsorption or a Dispersion subfeature to the **Porous Medium** to account for the corresponding transport mechanism.

Fluid (Porous Medium)

Use this node to specify the mass transfer in the mobile fluid solvent filling the pores of a porous medium. It is used as a subnode to Porous Medium.

MODEL INPUTS

The temperature model input is always available. By default, the **Temperature** model input is set to **Common model input**, and the temperature is controlled from Default Model Inputs under **Global Definitions** or by a locally defined Model Input. If a Heat

Transfer interface is included in the component, it controls the temperature **Common model input**. Alternatively, the temperature field can be selected from another physics interface. All physics interfaces have their own tags (**Name**). For example, if a Heat Transfer in Fluids interface is included in the component, the **Temperature (ht)** option is available for T.

You can also select **User defined** from the **Temperature** model input in order to manually prescribe T.

CONVECTION

If transport by convection is active, the velocity field of the solvent needs to be specified. For **User defined**, enter values or expressions for the velocity components in the input fields. This input option is always available. You can also select the velocity field solved for by a Fluid Flow interface added to the model component. These physics interfaces are available for selection in the **Velocity field** list.

DIFFUSION

Use this section to specify diffusion coefficients describing the diffusion of each species in the solvent fluid.

Use the **Source** list to select to pick up diffusion coefficients defined in a material or a Chemistry interface.

Select **Material**, and a **Fluid material** to use a diffusion coefficient in a material available in the model. User-defined property groups including a diffusion coefficient output property are available for selection in the **Fluid diffusion coefficient** list.

Select **Chemistry** to use a diffusion coefficient from a Chemistry interface added to model component. Diffusion coefficients are automatically defined when **Calculate transport properties** is selected on the interface level of a Chemistry interface. All defined diffusion coefficients are available for selection in the **Fluid diffusion coefficient** list.

For **User defined**, enter a value or expression for the **Fluid diffusion coefficient** $D_{\mathrm{F,i}}$ of each species in the corresponding input field.

In a porous medium the diffusivity is reduced due to the fact that the solid grains impede Brownian motion. Select an **Effective diffusivity model** to account for the reduced diffusivity. The available models are **Millington and Quirk model** (the default), **Bruggeman model**, **Tortuosity model**, or **No correction**. For **Tortuosity model**, enter a value for the tortuosity $\tau_{\mathrm{F,i}}$ (dimensionless).

Note that multiple species, as well as Migration in Electric fields (described below) is only available for certain COMSOL Multiphysics add-on products.For details, see https://www.comsol.com/products/specifications/.

MIGRATION IN ELECTRIC FIELD

This section is available when the **Migration in electric field** checkbox is selected. From the **Electric potential** list, select the source of the electric field.

- For **User defined**, enter a value or expression for the **Electric potential** V. This input option is always available.
- Select the electric potential solved by an AC/DC-based interface that has added to the component.
- Select the electric potential defined or solved for by an Electrochemistry interface added to the component.

By default the **Mobility** is set to be calculated based on the species effective diffusivity and the temperature using the **Nernst-Einstein relation**. For **User defined**, select the appropriate scalar or tensor type — **Isotropic**, **Diagonal**, **Symmetric**, or **Full** — and type in the value or expression of the effective mobility $u_{\mathrm{me,i}}$.

Enter the **Charge number** z_{c} for each species.

Porous Matrix

This node sets the porosity when modeling transport of diluted species in a Porous Medium or an Unsaturated Porous Medium. The porosity corresponds to the volume fraction occupied by the species containing fluid.

- By default the porosity of the solid matrix, ε_{p}, is taken **From material**. The **Porous Matrix** node supports the use of a **Porous Material** added to the Materials branch. In this case the porosity is defined in the manner of

$$\varepsilon_{\mathrm{p}} = 1 - \sum_i \theta_{\mathrm{s},i} - \sum_i \theta_{\mathrm{imf},i}$$

  where $\theta_{\mathrm{s},i}$ and $\theta_{\mathrm{imf},i}$ are the volume fractions given in **Solid** and **Immobile Fluids** subnodes under the **Porous Material** node.
- Select **From pellet bed densities** to compute the porosity using the (dry bulk) **Bed density** ρ_{b} and the (single phase) **Pellet density** ρ_{pe}. The porosity is then defined from

$$\varepsilon_p = 1 - \frac{\rho_b}{\rho_{pe}}$$

- For **User defined**, enter a value or expression for the porosity.

Dispersion

Local variations in the velocity as the fluid flows around solid particles lead to mechanical mixing, referred to as dispersion. Use this feature to account for dispersion in a Porous Medium or a Unsaturated Porous Medium

This subfeature is available when both the **Mass transfer in porous media mass transfer** checkbox and the **Convection** checkbox are selected in the **Settings** window for the physics interface.

Select the **Specify dispersion for each species individually** checkbox to specify the dispersion tensor D_D (SI unit: m^2/s) for each species separately. When not selected the same dispersion tensor D_D is used for all species.

Select an option from the **Dispersion tensor** list — **Dispersivity** or **User defined**.

Select **Dispersivity** to specify the dispersion in terms of dispersivities (SI unit: m). Select an option from the **Dispersivity model** list: **Isotropic** (the default) or **Transverse isotropic** based on the properties of the porous media. For isotropic porous media, specify the longitudinal and transverse dispersivities. For transverse isotropic porous media, specify the longitudinal, horizontal transverse, and vertical transverse dispersivities.

For **User defined**, specify the dispersion components in terms of constants or expressions. Select **Isotropic**, **Diagonal**, **Symmetric**, or **Full** to enable the appropriate tensor components.

Unsaturated Porous Medium

Use this node to model the concentration of diluted species transported by a solvent (mobile fluid phase) through interstices in a solid porous medium. In addition to transport due to convection and diffusion, the node contains functionality to include species evolution through adsorption and dispersion.

Use this node to model the concentration of diluted species transported by a liquid (mobile fluid phase) in a partially filled solid porous medium. The interstices of the porous medium contains the liquid carrier phase and gas pockets. Apart from

convection and diffusion, the node contains functionality to include species evolution through adsorption, dispersion, and volatilization.

!	This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

The properties of each phase present are defined using the Liquid, the Gas, and the Porous Matrix subnodes respectively. The Unsaturated Porous Medium node supports material properties using a Porous Material node, where properties are defined per phase in a similar manner.

Add an Adsorption or a Dispersion subfeature to the **Unsaturated Porous Medium** to account for the corresponding transport mechanism.

Liquid

Use this node to specify the mass transfer in the mobile liquid solvent present in the pores of the Unsaturated Porous Medium.

MODEL INPUTS

The temperature model input is always available. By default, the **Temperature** model input is set to **Common model input**, and the temperature is controlled from Default Model Inputs under **Global Definitions** or by a locally defined Model Input. If a Heat Transfer interface is included in the component, it controls the temperature **Common model input**. Alternatively, the temperature field can be selected from another physics interface. All physics interfaces have their own tags (**Name**). For example, if a Heat Transfer in Fluids interface is included in the component, the **Temperature (ht)** option is available for T.

You can also select **User defined** from the **Temperature** model input in order to manually prescribe T.

SATURATION

Select **Saturation** or **Liquid volume fraction** from the list.

For **Saturation**, enter a value for s (dimensionless) between 0 and 1. The liquid volume fraction is then computed from the saturation and porosity as $\theta_l = \varepsilon_p s$.

For **Liquid volume fraction**, enter a value for θ_l (dimensionless) between 0 and the value of the porosity.

Select a **Liquid fraction time change**: **Liquid fraction constant in time** (the default), **Time change in liquid fraction**, or **Time change in pressure head**.

- For **Time change in fluid fraction**, enter $\mathrm{d}\theta/\mathrm{d}t$ (SI unit: 1/s).
- For **Time change in pressure head**, enter $\mathrm{d}H_\mathrm{p}/\mathrm{d}t$ (SI unit: m/s) and a **Specific moisture capacity** C_m (SI unit: 1/m). If a Darcy's Law interface is included in the component, the time change in pressure head solved for can be selected.

CONVECTION

If transport by convection is active, the velocity field of the solvent needs to be specified. For **User defined**, enter values or expressions for the velocity components in the input fields. This input option is always available. You can also select the velocity field solved for by a Fluid Flow interface added to the model component. These physics interfaces are available for selection in the **Velocity field** list.

DIFFUSION

Use this section to specify diffusion coefficients describing the diffusion of each species in the solvent liquid.

Use the **Source** list to select to pick up diffusion coefficients defined in a material or a Chemistry interface.

Select **Material**, and a **Liquid material** to use a diffusion coefficient in a material available in the model. User-defined property groups including a diffusion coefficient output property are available for selection in the **Liquid diffusion coefficient** list.

Select **Chemistry** to use a diffusion coefficient from a Chemistry interface added to model component. Diffusion coefficients are automatically defined when **Calculate transport properties** is selected on the interface level of a Chemistry interface. All defined diffusion coefficients are available for selection in the **Liquid diffusion coefficient** list.

For **User defined**, enter a value or expression for the **Liquid diffusion coefficient** $D_\mathrm{L,i}$ of each species in the corresponding input field.

In a porous medium the diffusivity is reduced due to the fact that the solid grains impede Brownian motion. Select an **Effective diffusivity model, liquid** to account for the reduced diffusivity in the liquid. The available models are **Millington and Quirk model**

(the default), **Bruggeman model**, **Tortuosity model**, or **No correction**. For **Tortuosity model**, enter a value for the tortuosity $\tau_{L,i}$ (dimensionless).

Note that multiple species, as well as Migration in Electric fields (described below) is only available for certain COMSOL Multiphysics add-on products. For details see: https://www.comsol.com/products/specifications/.

MIGRATION IN ELECTRIC FIELD

This section is available when the **Migration in electric field** checkbox is selected. From the **Electric potential** list, select the source of the electric field.

- For **User defined**, enter a value or expression for the **Electric potential** V. This input option is always available.
- Select the electric potential solved by an AC/DC-based interface that has added to the component.
- Select the electric potential defined or solved for by an Electrochemistry interface added to the component.

By default the **Mobility** is set to be calculated based on the species effective diffusivity and the temperature using the **Nernst-Einstein relation**. For **User defined**, select the appropriate scalar or tensor type — **Isotropic**, **Diagonal**, **Symmetric**, or **Full** — and type in the value or expression of the effective mobility $u_{me,i}$.

Enter the **Charge number** z_c for each species.

Gas

Use this node to specify the mass transfer in the gas phase present in the pores of the Unsaturated Porous Medium.

DIFFUSION

The settings for the diffusion of each species in the gas phase are identical to those in the Liquid subnode.

VOLATILIZATION

Enter a value for the volatilization isotherm $k_{G,c}$ (dimensionless) for each species.

Adsorption

Use this node to model adsorption of the (fluid phase) solute species onto the surface of the porous matrix. It is available as a subnode to the Porous Medium and the Unsaturated Porous Medium nodes.

!	This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

MATRIX PROPERTIES

The density of the porous media is needed when modeling adsorption to the surface of the porous matrix. Choose to input either the **Dry bulk density** ρ, or the **Solid phase density** ρ_s. The former is the density of the porous matrix including empty pores, while the latter corresponds to the density of the pure solid phase. The density can be defined from the domain material by selecting **From material**, or from a user defined expression. When a **Porous Material** is used on the selection, the density will be requested from a **Solid** subfeature. Several **Solid** features can be used to model a homogeneous mixture of several solid components.

ADSORPTION

Select an **Adsorption isotherm** — **Langmuir**, **Freundlich**, **Toth**, **BET**, or **User defined** to specify how to compute c_P, the amount of species sorbed to the solid phase (moles per unit dry weight of the solid):

- For **Langmuir**:

$$c_P = c_{Pmax}\frac{K_L c}{1 + K_L c} \quad , \quad K_P = \frac{\partial c_P}{\partial c} = \frac{K_L c_{Pmax}}{(1 + K_L c)^2}$$

  Enter a **Langmuir constant** $k_{L,c}$ (SI unit: m^3/mol) and an **Adsorption maximum** $c_{p,max,c}$ (SI unit: mol/kg).

- For **Freundlich**:

$$c_P = K_F\left(\frac{c}{c_{ref}}\right)^N \quad , \quad K_P = \frac{\partial c_P}{\partial c} = N\frac{c_P}{c}$$

Enter a **Freundlich constant** $k_{F,c}$ (SI unit: mol/kg), a **Freundlich exponent** $N_{F,c}$ (dimensionless), and a **Reference concentration** $c_{ref,c}$ (SI unit: mol/m^3).

- For **Toth**:

$$c_P = c_{Pmax}\frac{b_T c}{(1+(b_T c)^{N_T})^{1/N_T}}$$

and

$$K_P = \frac{\partial c_P}{\partial c} = c_{Pmax} b_T (1+(b_T c)^{N_T})^{-\left(1+\frac{1}{N_T}\right)}$$

Enter a **Toth constant** $b_{T,c}$ (SI unit: m^3/mol), a **Toth exponent** $N_{T,c}$ (dimensionless), and an **Adsorption maximum** $c_{p,max,c}$ (SI unit: mol/kg).

- For **BET (Brunauer-Emmett-Teller)**:

$$c_P = \frac{K_B c_0 c}{(c_S - c)\left(1+(K_B-1)\frac{c}{c_S}\right)}$$

and

$$K_P = \frac{\partial c_P}{\partial c} = \frac{K_B c_0 c_S((K_B-1)c^2 + c_S^2)}{(c-c_S)^2(c_S+(K_B-1)c)^2}$$

Enter a **BET constant** $K_{B,c}$ (dimensionless), a **Monolayer adsorption capacity** $c_{0,c}$ (SI unit: mol/kg), and an **Saturation concentration** $c_{S,c}$ (SI unit: mol/m^3).

- For **User defined** enter an **Adsorption isotherm** $c_{P,c}$ (SI unit: mol/kg):

$$c_P = f(c)$$

For more information, see Adsorption in the theory section.

FURTHER READING

See the theory chapter in the section Mass Balance Equation for Transport of Diluted Species in Porous Media.

Volatilization

This feature is available when the **Mass transfer in porous media** checkbox is selected in the **Settings** window for the physics interface.

Use this feature to model mass transfer at the boundary due to volatilization. The species dissolved in the liquid are assumed to be vaporized at the boundary, and transported into the surrounding bulk region due to convection and diffusion. The mass transfer at the boundary is defined as

$$-\mathbf{n} \cdot \mathbf{J}_{\mathrm{c}} = -h_{\mathrm{c}}(k_{\mathrm{G,c}}c - c_{\mathrm{Gatm,c}})$$

where h_{c} is the mass transfer coefficient, $k_{\mathrm{G,c}}$ the volatilization coefficient, and $c_{\mathrm{Gatm,c}}$ the concentration in the surrounding atmosphere.

!	This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

VOLATILIZATION

Enter a **Mass transfer coefficient** h_{c} defining the transfer into the surrounding media. This can be given by boundary layer theory. When assuming that no convective flow is present in the surrounding, the mass transfer coefficient can be defined from the gas diffusion coefficient D_{Gc} and the thickness of the diffusion layer d_{s} in the manner of

$$h_{\mathrm{c}} = \frac{D_{\mathrm{Gc}}}{d_{\mathrm{s}}}$$

Also give the atmospheric concentration for each species, $c_{\mathrm{Gatm,c}}$. The **Volatilization** coefficient $k_{\mathrm{G,c}}$ for each species are taken from the adjacent Unsaturated Porous Medium domain.

Species Source

In order to account for consumption or production of species in porous domains, the **Species Source** node adds source terms expressions S_i to the right-hand side of the species transport equations.

DOMAIN SELECTION

From the **Selection** list, choose the domains on which to define rate expression or expressions that govern the source term in the transport equations.

If there are several types of domains, with subsequent and different reactions occurring within them, it might be necessary to remove some domains from the selection. These are then defined in an additional **Species Source** node.

SPECIES SOURCE

Add a source term S_i (SI unit: mol/(m^3·s)) for each of the species solved for. Enter a value or expression in the field of the corresponding species.

Hygroscopic Swelling

The **Hygroscopic Swelling** multiphysics coupling node ( ) is used for moisture concentration coupling between the Solid Mechanics interface and either the Transport of Diluted Species or Transport of Diluted Species in Porous Media interfaces.

Hygroscopic swelling is an effect of internal strain caused by changes in moisture content. This volumetric strain can be written as

$$\varepsilon_{\mathrm{hs}} = \beta_{\mathrm{h}} M_{\mathrm{m}} (c_{\mathrm{mo}} - c_{\mathrm{mo,ref}})$$

where β_{h} is the coefficient of hygroscopic swelling, M_{m} is the molar mass, c_{mo} is the moisture concentration, and $c_{\mathrm{mo,ref}}$ is the strain-free reference concentration.

This feature requires a license of either the MEMS Module or the Structural Mechanics Module. The multiphysics feature will appear automatically if both the Transport of Diluted Species and the Solid Mechanics interfaces are added to the same component. For the most current information about licensing, please see https://www.comsol.com/products/specifications/.

FURTHER READING

More information about how to use hygroscopic swelling can be found in the Hygroscopic Swelling section in the *Structural Mechanics Module User's Guide*.

More information about multiphysics coupling nodes can be found in the section The Multiphysics Branch.

Out-of-Plane Flux

The out-of-plane flux node is used to prescribe a flux in an out-of-plane domain, and it can be used to reduce a model geometry to 2D, or even 1D, when the concentration variation is small in one or more directions. This could be the case for example when the object to model is thin or slender. Figure 8-1 shows examples of possible situations in which this type of geometry reduction can be applied.

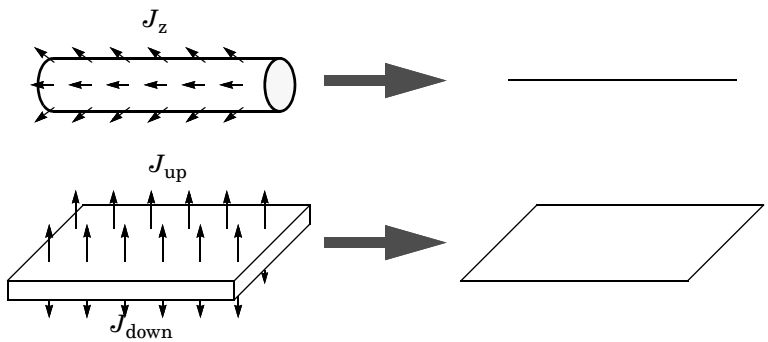


Figure 8-1: Geometry reduction from 3D to 1D (top) and from 3D to 2D (bottom).

For a 1D component this node adds a single out-of-plane molar flux $J_{0,z,i}$ for species i. For a 2D component two fluxes can be prescribed for each species; $J_{0,u,i}$ for the upside of the domain, and $J_{0,d,i}$ for the downside of the domain.

The fluxes are added as a source contribution to the right-hand side of the transport equation. For example, in 2D components with diffusion, convection, and out-of-plane flux present, the mass transfer of species i is defined by the mass conservation equation

$$\frac{\partial c_i}{\partial t} + \nabla \cdot \mathbf{J}_i + \mathbf{u} \cdot \nabla c_i = R_i + S_{\mathrm{opf},i}, \tag{8-1}$$

where $S_{\mathrm{opf},i}$ is the out-of-plane source for species i

$$S_{\mathrm{opf},i} = \frac{J_{0,i}}{d_z} = \frac{J_{0,\mathrm{u},i} + J_{0,\mathrm{d},i}}{d_z}.$$

For external convection on the upside and the downside of the domain, the out-of-plane flux is

$$J_{0,i} = k_{\mathrm{c,u},i}(c_{\mathrm{b,u},i} - c_i) + k_{\mathrm{c,d},i}(c_{\mathrm{b,d},i} - c_i)$$

where k_c is a mass transfer coefficient and c_b is the bulk concentration, the typical concentration far into the surrounding exterior domain. The prescribed flux, J_0, can include any arbitrary user-specified expressions. It can be a constant or a function of a dependent variable or independent variables.

UPSIDE INWARD FLUX

For 1D components, enter the **cross-sectional perimeter** $\mathrm{P_c}$ to get the out-of-plane flux

$$J_{0,i} = P_c J_{0,\mathrm{z},i}.$$

The default value of P_c is the circumference. Either keep the default value, for a circular cross-section shape, or edit the value to get a user-defined shape of the out-of-plane cross-section.

The available flux type options are **General inward flux** and **External convection**. Select the **Species** checkbox for the species for which to specify the flux, and enter a value or expression for the inward flux in the corresponding field. Use a minus sign when specifying a flux directed out of the system. To use another boundary condition for a specific species, click to clear the checkbox for that species.

Set **Flux type** to **External convection** to prescribe a flux to or from an exterior domain (not modeled) assumed to include convection. The exterior can for example include a forced convection to control the temperature or to increase the mass transport. In this case the prescribed mass flux corresponds to

$$J_0 = k_\mathrm{c}(c_\mathrm{b} - c)$$

where k_c is a mass transfer coefficient and c_b is the bulk concentration, the typical concentration far into the surrounding exterior domain.

DOWNSIDE INWARD FLUX

The available options are **General inward flux** and **External convection**. The settings are the same as for the Upside Inward Flux section.

FURTHER READING

For an example of using the Out-of-Plane Flux node, see this application example:

	Cross-Flow Mass Transfer in a Thin Domain: Application Library path **Chemical_Reaction_Engineering_Module/Tutorials/thin_domain**

Fracture

Use this node to model mass transport along thin fractures in porous media. The node assumes that the transport in the tangential direction along the fracture is dominant as a result of lower flow resistance.

The Fracture feature has two default subfeatures — the Fluid (Fracture) subfeature where convection and diffusion are specified and the Fracture Material subfeature where the porosity ε_p is defined.

!	This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

FRACTURE PROPERTIES

Specify a value for the **Fracture thickness** d_{fr}.

For the **Fracture** boundary condition, there are a number of **Attributes** available which can be accessed either via the **Physics** Ribbon toolbar (for Windows) or by right-clicking on the **Fracture** node. These attributes are identical to the Boundary, Edge, Point, and Pair Nodes for the Transport of Diluted Species in Fractures Interface described, for example, in the *Chemical Reaction Engineering Module User's Guide*.

Fluid (Fracture)

Use this node to specify the mass transfer in the mobile fluid solvent filling the pores of a fracture.

It uses the same input options as the Fluid (Porous Medium) subfeature under the Porous Medium feature. There are further details about the settings.

MODEL INPUTS

The temperature model input is always available. By default, the **Temperature** model input is set to **Common model input**, and the temperature is controlled from **Default Model Inputs** under **Global Definitions** or by a locally defined **Model Input**. If a Heat Transfer interface is included in the component, it controls the temperature **Common model input**. Alternatively, the temperature field can be selected from another physics interface. All physics interfaces have their own tags (**Name**). For example, if a Heat Transfer in Fluids interface is included in the component, the **Temperature (ht)** option is available for T.

CONVECTION

If transport by convection is active, the velocity field of the solvent needs to be specified. Select an option from the **Velocity field** list to specify the convective velocity along the fracture. For a consistent model, use a Fracture feature in a Darcy's Law interface to compute the fluid flow velocity in the fracture.

For **User defined**, enter values or expressions for the velocity components in the table shown

DIFFUSION

Use this section to specify diffusion coefficients describing the diffusion of each species in the solvent fluid.

The **Diffusion** settings are similar to those for the diffusion coefficients in the Fluid (Porous Medium) node under Porous Medium.

Fracture Material

Specify the **Porosity** ε_p (dimensionless) of the porous matrix. This is by default taken **From material**. Select **From pellet bed densities** to compute the porosity from the (dry bulk) **Bed density** ρ_b and the (single phase) **Pellet density** ρ_{pe} through the relation

$$\varepsilon_p = 1 - \frac{\rho_b}{\rho_{pe}}$$

For **User defined**, enter a value or expression for the porosity.

Theory for the Transport of Diluted Species Interface

The Transport of Diluted Species Interface provides a predefined modeling environment for studying the evolution of chemical species transported by diffusion and convection as well as migration due to an electric field. The physics interface assumes that all species present are dilute; that is, that their concentration is low compared to a solvent fluid or solid. As a rule of thumb, a mixture containing several species can be considered dilute when the concentration of the solvent is more than 90 mol%. Due to the dilution, mixture properties such as density and viscosity can be assumed to correspond to those of the solvent.

When studying mixtures that are not dilute, the mixture and transport properties depend on the composition, and a different physics interface is recommended. See The Transport of Concentrated Species Interface in the *Chemical Reaction Engineering Module User's Guide* for more information.

Fick's law governs the diffusion of the solutes, dilute mixtures, or solutions, while the phenomenon of ionic migration is sometimes referred to as *electrokinetic flow*. The Transport of Diluted Species interface supports the simulations of chemical species transport by convection, migration, and diffusion in 1D, 2D, and 3D as well as for axisymmetric components in 1D and 2D.

In this section:

- Adding Transport Through Migration
- Material Balance Formulation
- Crosswind Diffusion
- Danckwerts Inflow Boundary Condition
- Equilibrium Reaction Theory
- Mass Balance Equation
- Mass Sources for Species Transport
- Solving a Diffusion Equation Only
- Supporting Electrolytes
- References

Note: Some features explained in this section require certain add-on modules. For details see https://www.comsol.com/products/specifications/

The section also includes the theory for The Transport of Diluted Species in Porous Media Interface:

- Adsorption
- Convection in Porous Media
- Diffusion in Porous Media
- Dispersion
- Mass Balance Equation for Transport of Diluted Species in Porous Media
- Mass Transport in Fractures
- Reactions

Mass Balance Equation

The default node attributed to the Transport of Diluted Species interface models chemical species transport through diffusion and convection and solves the mass conservation equation for one or more chemical species i:

$$\frac{\partial c_i}{\partial t} + \nabla \cdot \mathbf{J}_i + \mathbf{u} \cdot \nabla c_i = R_i \tag{8-2}$$

Equation 8-2 in its form above includes the transport mechanisms diffusion and convection. If *Migration in Electric Field* is activated (only available in some add-on products), the migration mechanism will be added to the equation as well. See more details in the section Adding Transport Through Migration.

- c_i is the concentration of the species (SI unit: mol/m^3)
- D_i denotes the diffusion coefficient (SI unit: m^2/s)
- R_i is a reaction rate expression for the species (SI unit: mol/(m^3·s))
- $\mathbf{u}$ is the mass averaged velocity vector (SI unit: m/s)
- $\mathbf{J}_i$ is the mass flux diffusive flux vector (SI unit: mol/(m^2·s))

The mass flux relative to the mass averaged velocity, $\mathbf{J}_i$ (SI unit: mol/(m^2·s)), is associated with the mass balance equation above and used in boundary conditions and flux computations. The Transport of Diluted Species interface always includes mass transport due to molecular diffusion. In this case the mass flux $\mathbf{J}_i$ defines the diffusive flux vector

$$\mathbf{J}_i = -D\nabla c_i \tag{8-3}$$

An input field for the diffusion coefficient is available.

When *Migration in Electric Fields* is activated, the migration term is also added to the diffusive flux vector as shown in the section Adding Transport Through Migration.

The third term on the left side of Equation 8-2 describes the convective transport due to a velocity field **u**. This field can be expressed analytically or obtained from coupling the physics interface to one that solves for fluid flow, such as *Laminar Flow*. Note that all fluid flow interfaces solve for the mass averaged velocity.

On the right-hand side of the mass balance equation (Equation 8-2), R_i represents a source or sink term, typically due to a chemical reaction or desorption on a porous matrix. To specify R_i, another node must be added to the Transport of Diluted Species interface — the **Reaction** node for example, which includes an input field for specifying a reaction expression using the variable names of all participating species.

Equilibrium Reaction Theory

The feature Equilibrium Reaction is described in this section. A chemical equilibrium reaction system is defined by the stoichiometry of the reaction and the relation between the chemical activities of the chemical species participating in the reaction (the equilibrium condition).

The kinetics of the reaction is so fast that the equilibrium condition is fulfilled at all times in all space coordinates.

The equilibrium condition is commonly based on the stoichiometric coefficients, ν_i (dimensionless), of the reaction; the species activities of the reacting species a_i (dimensionless); and an equilibrium constant, K_{eq} (1) according to

$$K_{\mathrm{eq}} = \frac{\prod_{i \in \text{ products}} a_i^{\nu_i}}{\prod_{i \in \text{ reactants}} a_i^{-\nu_i}}$$

where the species activities are defined as

$$a_i = \gamma_{c,i} \frac{c_i}{c_{\mathrm{a0}}}$$

where c_{a0} (SI unit: mol/m^3) is the standard molarity, and $\gamma_{c,i}$ (dimensionless) an activity coefficient.

Defining the stoichiometric coefficients positive for products and negative for reactants, the above equilibrium condition can also be written

$$K_{\mathrm{eq}} = \prod_i a_i^{\nu_i}$$

The Equilibrium Reaction node solves for a reaction rate so that the equilibrium condition is always fulfilled in the domain. It is available for the Chemical Reaction Engineering Module; Battery Design Module; Corrosion Module; Electrochemistry Module; Electrodeposition Module; and Fuel Cell & Electrolyzer Module.

	$\gamma_{c,i}$ is set to unity when the Equilibrium constant is selected in the Settings window. For nonunity activity coefficients, a user-defined equilibrium condition can be used.

EQUILIBRIUM REACTIONS AND INFLOW BOUNDARY CONDITIONS

Contradictory constraints arise if the boundary conditions for concentrations or activities are set so that the domain equilibrium condition is not fulfilled. Special treatment is therefore needed at Inflow boundaries, where the concentrations are set for all species in the mass transport interfaces.

One way of avoiding competing constraints on an inflow boundary is to add an additional reaction coordinate degree of freedom, solved for to create a set of modified inflow concentrations that fulfill the domain equilibrium condition. The reaction coordinate gives rise to a concentration shift, which is the offset to the inflow concentrations provided by the user. The shift for each species obeys the stoichiometry of the reaction and the equilibrium expression. The modified inflow concentrations are then used in the boundary conditions for the domain mass transport equations. The resulting modified inflow concentrations can be seen as the stationary solution for a batch reactor with the user inflow concentrations as initial concentrations. In addition, the domain reaction rate degree of freedom of the equilibrium reaction is constrained to zero on all Inflow boundaries.

EQUILIBRIUM REACTIONS AND CONCENTRATION BOUNDARY CONDITIONS

No special treatment is made with regards to input concentration values of the Concentration boundary node. Using this feature, you can explicitly set one or a set of concentrations, and the equilibrium condition acts on the rest of the concentrations.

However, there is no solution to the problem if more concentrations than the number of species minus the number of equilibrium reactions are set using this feature.

EQUILIBRIUM REACTIONS AND TIME-DEPENDENT SIMULATIONS

Spurious oscillations may occur in a time-dependent problem if the initial conditions do not fulfill the equilibrium condition. Since equilibrium reactions are assumed to be infinitely fast, the solution is to initialize the problem using an additional study step, solving for a stationary problem with all nonequilibrium reaction rates set to zero. Manual scaling of the reaction rate dependent variables is needed in this study step.

Material Balance Formulation

The default node attributed to The Transport of Diluted Species Interface assumes chemical species transport through diffusion and convection (depending on the modules licensed, a checkbox to activate migration is available) and implements the mass balance equation in Equation 8-2.

Two formulations of the mass balance are available, these are referred to as the nonconservative and conservative form:

$$\text{nonconservative: } \frac{\partial c}{\partial t} + \nabla \cdot \mathbf{J}_i + \mathbf{u} \cdot \nabla c = R \tag{8-4}$$

$$\text{conservative: } \frac{\partial c}{\partial t} + \nabla \cdot \mathbf{J}_i + \nabla \cdot (c\mathbf{u}) = R \tag{8-5}$$

In these equations $\mathbf{J}_i$ is the diffusive flux vector, $\mathbf{u}$ is the solvent velocity field, and R is a production or consumption rate expression. The nonconservative is often more numerically robust, and therefore chosen by default for the interface. This formulation however disregards density changes in the fluid. This can be seen by expanding the conservative convection term using the chain rule. One of the resulting terms, $c\nabla\cdot\mathbf{u}$, equals zero for an incompressible fluid which results in the nonconservative form. To switch between the two formulations, click the **Show** button ( ) and select **Advanced Physics Options**.

Solving a Diffusion Equation Only

Remove the convection term from Equation 8-4 and Equation 8-5 by clearing the Convection checkbox in the Transport Mechanisms section for The Transport of Diluted Species Interface. The equation then becomes

$$\frac{\partial c}{\partial t} = \nabla \cdot \mathbf{J}_i + R$$

Mass Sources for Species Transport

Note: The features below are only available in a limited set of add-on products. For a detailed overview of which features are available in each product, visit https://www.comsol.com/products/specifications/

There are two types of mass sources in the Transport of Diluted Species interface: point sources and line sources.

POINT SOURCE

A point source is theoretically formed by assuming a mass injection/ejection, Q_c (SI unit: mol/(m^3·s)), in a small volume δV and then letting the size of the volume tend to zero while keeping the total mass flux constant. Given a point source strength, $\dot{q}_{p,c}$ (SI unit: mol/s), this can be expressed as

$$\lim_{\delta V \to 0} \int_{\delta V} Q_c = \dot{q}_{p,c} \tag{8-6}$$

An alternative way to form a point source is to assume that mass is injected/extracted through the surface of a small object. Letting the object surface area tend to zero while keeping the mass flux constant results in the same point source. For this alternative approach, effects resulting from the physical object's volume need to be neglected.

The weak contribution

$$\dot{q}_{p,c}\mathrm{test}(c)$$

is added at a point in the geometry. As can be seen from Equation 8-6, Q_c must tend to plus or minus infinity as δV tends to zero. This means that in theory the concentration also tends to plus or minus infinity.

Observe that "point" refers to the physical representation of the source. A point source can therefore only be added to points in 3D components and to points on the symmetry axis in 2D axisymmetry components. Other geometrical points in 2D components represent physical lines.

The finite element representation of Equation 8-6 corresponds to a finite concentration at a point with the effect of the point source spread out over a region around the point. The size of the region depends on the mesh and on the strength of the source. A finer mesh gives a smaller affected region but also a more extreme concentration value. It is important not to mesh too finely around a point source since this can result in unphysical concentration values. It can also have a negative effect on the condition number for the equation system.

LINE SOURCE

A line source can theoretically be formed by assuming a source of strength $\dot{Q}_{l,c}$ (SI unit: mol/(m^3·s)), located within a tube with cross section δS and then letting δS tend to zero while keeping the total mass flux per unit length constant. Given a line source strength, $\dot{q}_{l,c}$ (SI unit: mol/(m·s)), this can be expressed as

$$\lim_{\delta S \to 0} \int_{\delta S} \dot{Q}_{l,c} = \dot{q}_{l,c} \tag{8-7}$$

As in the point source case, an alternative approach is to assume that mass is injected/extracted through the surface of a small object. This results in the same mass source, but requires that effects resulting from the physical object's volume are neglected.

The weak contribution

$$\dot{q}_{l,c}\mathrm{test}(c)$$

is added on lines in 3D or at points in 2D (which represent cut-through views of lines). Line sources can also be added on the axisymmetry line in 2D axisymmetry components. It cannot, however, be added on geometrical lines in 2D since those represent physical planes.

As with a point source, it is important not to mesh too finely around the line source.

	For feature node information, see Line Mass Source and Point Mass Source.

Adding Transport Through Migration

Note: Migration is only available in a limited set of add-on products. For a detailed overview of which features are available in each product, visit https://www.comsol.com/products/specifications/

In addition to transport due to convection and diffusion, the Transport of Diluted Species interface supports ionic species transport by *migration*. This is done by selecting the Migration in Electric Field checkbox under the Transport Mechanisms section for the physics interface. The mass balance then becomes:

$$\frac{\partial c_i}{\partial t} + \nabla \cdot (-D_i \nabla c_i - z_i u_{\mathrm{m},i} F c_i \nabla V + c_i \mathbf{u}) = R_i \tag{8-8}$$

where

- c_i (SI unit: mol/ m^3) denotes the concentration of species i
- D_i (SI unit: m^2/s) is the diffusion coefficient of species i
- $\mathbf{u}$ (SI unit: m/s) is the fluid velocity
- F (SI unit: A·s/mol) refers to Faraday's constant
- V (SI unit: V) denotes the electric potential
- z_i (dimensionless) is the charge number of the ionic species, and
- $u_{\mathrm{m},i}$ (SI unit: mol·s/kg) is its ionic mobility

In this case the diffusive flux vector is

$$\mathbf{J}_i = -D_i \nabla c_i - z_i u_{\mathrm{m},i} F c_i \nabla V$$

The velocity, $\mathbf{u}$, can be a computed fluid velocity field from a Fluid Flow interface or a specified function of the spatial variables x, y, and z. The potential can be provided by an expression or by coupling the system of equations to a current balance, such as the Electrostatics interface. Sometimes it is assumed to be a supporting electrolyte present, which simplifies the transport equations. In that case, the modeled charged species concentration is very low compared to other ions dissolved in the solution. Thus, the species concentration does not influence the solution's conductivity and the net charge within the fluid.

The Nernst–Einstein relation can in many cases be used for relating the species mobility to the species diffusivity according to

$$u_{m,i} = \frac{D_i}{RT}$$

where R (SI unit: J/(mol·K)) is the molar gas constant and T (SI unit: K) is the temperature.

Note: In the *Nernst–Planck Equations* interface, the ionic species contribute to the charge transfer in the solution. It includes an *electroneutrality condition* and also computes the electric potential field in the electrolyte. For more information, see Theory for the Nernst–Planck Equations Interface. This interface is included in the Chemical Reaction Engineering Module.

Supporting Electrolytes

In *electrolyte* solutions, a salt can be added to provide a high electrolyte conductivity and decrease the ohmic losses in a cell. These solutions are often called *supporting electrolytes*, buffer solutions, or carrier electrolytes. The added species, a negative and a positive ion pair, predominates over all other species. Therefore, the supporting electrolyte species can be assumed to dominate the current transport in the solution. In addition, the predominant supporting ions are usually selected so that they do not react at the electrode surfaces since the high conductivity should be kept through the process, that is, they should not be electroactive species. This also means that the concentration gradients of the predominant species in a supporting electrolyte are usually negligible.

Modeling and solving for a supporting electrolyte in the *Electrostatics* or *Secondary Current Distribution* interfaces will give a potential distribution that drives the migration in the Transport of Diluted Species Interface.

The current density vector is proportional to the sum of all species fluxes as expressed by Faraday's law:

$$\mathbf{i} = F\sum_i z_i \mathbf{N}_i$$

The electroneutrality condition ensures that there is always a zero net charge at any position in a dilute solution. Intuitively, this means that it is impossible to create a current by manually pumping positive ions in one direction and negative ions in the other. Therefore, the convective term is canceled out to yield the following expression for the electrolyte current density, where j denotes the supporting species:

$$\mathbf{i} = F\sum_j -z_j^2 u_{\mathrm{m},j} F c_j \nabla\phi \tag{8-9}$$

Equation 8-9 is simply Ohm's law for ionic current transport and can be simplified to

$$\mathbf{i} = -\kappa\nabla\phi \tag{8-10}$$

where κ is the conductivity of the supporting electrolyte. A current balance gives the current and potential density in the cell

$$\nabla\cdot\mathbf{i} = 0$$

which, in combination with Equation 8-10, yields:

$$\nabla\cdot(-\kappa\nabla\phi) = 0 \tag{8-11}$$

Equation 8-11 can be easily solved using the Electrostatics or Secondary Current Distribution interface and, when coupled to the Transport in Diluted Species interface, the potential distribution shows up in the migration term.

Crosswind Diffusion

Transport of diluted species applications can often result in models with a very high cell Péclet number — that is, systems where convection or migration dominates over diffusion. Streamline diffusion and crosswind diffusion are of paramount importance to obtain physically reasonable results. The Transport of Diluted Species interface provides two crosswind diffusion options using different formulations. Observe that crosswind diffusion makes the equation system nonlinear even if the transport equation is linear.

DO CARMO AND GALEÃO

This is the formulation described in Numerical Stabilization in the *COMSOL Multiphysics Reference Manual*. The method reduces over- and undershoots to a minimum, even for anisotropic meshes.

In some cases, the resulting nonlinear equation system can be difficult to converge. This can happen when the cell Péclet number is very high and the model contains many thin layers, such as contact discontinuities. You then have three options:

- Refine the mesh, especially in regions with thin layers.
- Use a nonlinear solver with a constant damping factor less than one.
- Switch to the Codina crosswind formulation.

CODINA

The Codina formulation is described in Ref. 1. It adds diffusion strictly in the direction orthogonal to the streamline direction. Compared to the do Carmo and Galeão formulation, the Codina formulation adds less diffusion but is not as efficient at reducing over- and undershoots. It also does not work as well for anisotropic meshes. The advantage is that the resulting nonlinear system is easier to converge and that underresolved gradients are less smeared out.

Danckwerts Inflow Boundary Condition

Constraining the composition to fixed values at an inlet to a reactor may sometimes result in issues with unreasonably high reaction rates or singularities at the inlet boundary. These problems may many times be mitigated by using a flux boundary condition instead, based on the upstream concentrations and the fluid velocity at the boundary. In chemical engineering, this type of flux boundary condition is also known as a Danckwerts condition.

Use the Danckwerts condition to specify inlet conditions for domains where high reaction rates are anticipated in the vicinity to the inlet (Ref. 2).

Given an upstream concentration $c_{i,0}$, the Danckwerts inflow boundary condition prescribed the total flux as

$$\mathbf{n} \cdot (\mathbf{J}_i + \mathbf{u}c_i) = \mathbf{n} \cdot (\mathbf{u}c_{i,0}) \tag{8-12}$$

Mass Balance Equation for Transport of Diluted Species in Porous Media

VARIABLY SATURATED POROUS MEDIA

The following equations for the molar concentrations, c_i, describe the transport of solutes in a variably saturated porous medium for the most general case, when the pore space is primarily filled with liquid but also contain pockets or immobile gas:

$$\frac{\partial}{\partial t}(\theta_l c_i) + \frac{\partial}{\partial t}(\rho c_{P,i}) + \frac{\partial}{\partial t}(\theta_g c_{G,i}) + \mathbf{u} \cdot \nabla c_i = \nabla \cdot [(D_{D,i} + D_{e,i})\nabla c_i] + R_i + S_i \tag{8-13}$$

On the left-hand side of Equation 8-13, the first three terms correspond to the accumulation of species within the liquid, solid, and gas phases, while the last term describes the convection due to the velocity field $\mathbf{u}$ (SI unit: m/s).

In Equation 8-13 c_i denotes the concentration of species i in the liquid (SI unit: mol/m^3), $c_{P,i}$ the amount adsorbed to solid particles (moles per unit dry weight of the solid), and $c_{G,i}$ the concentration of species i in the gas phase.

The equation balances the mass transport throughout the porous medium using the porosity ε_p, the liquid volume fraction θ_l; the dry bulk density, $\rho = (1 - \varepsilon_p)\rho_s$, and the solid phase density ρ_s.

For saturated porous media, the liquid volume fraction θ_l is equal to the porosity ε_p, but for unsaturated porous media, they are related by the saturation s as $\theta_l = \varepsilon_p s$. The resulting gas volume fraction in the case of an unsaturated porous medium is

$$\theta_g = \varepsilon_p - \theta_l = (1 - s)\varepsilon_p$$

On the right-hand side of Equation 8-13, the first term introduces the spreading of species due to mechanical mixing resulting from the porous media (dispersion), as well as from diffusion and volatilization to the gas phase. The dispersion tensor is denoted D_D (SI unit: m^2/s) and the effective diffusion by D_e (SI unit: m^2/s).

The last two terms on the right-hand side of Equation 8-13 describe production or consumption of the species; R_i is a reaction rate expression which can account for reactions in the liquid, solid, or gas phase, and S_i is an arbitrary source term, for example due to a fluid flow source or sink.

Adsorption

The time evolution of the adsorption, the solute transport to or from the solid phase, is defined by assuming that the amount of solute adsorbed to the solid, $c_{P,i}$, is a function of the concentration in the fluid c_i. This implies that the solute concentration in the liquid and solid phase are in instant equilibrium. The adsorption term can be expanded to give

$$\frac{\partial}{\partial t}(\rho c_{P,i}) = \rho\frac{\partial c_{P,i}}{\partial c_i}\frac{\partial c_i}{\partial t} - c_{P,i}\rho_s\frac{\partial \varepsilon_p}{\partial t} = \rho K_{P,i}\frac{\partial c_i}{\partial t} - c_{P,i}\rho_s\frac{\partial \varepsilon_p}{\partial t} \tag{8-14}$$

where $K_{P,i} = \partial c_{P,i}/\partial c_i$ is the adsorption isotherm.

Volatilization

Volatilization is the process where a solute species in the liquid is transported to the gas phase due to vaporization. Assuming that the amount of solute in the gas phase, $c_{G,i}$, is a linear function of the liquid phase concentration, the volatilization term is defined as

$$\frac{\partial}{\partial t}\theta_g c_{G,i} = \theta_g\frac{\partial c_{G,i}}{\partial c_i}\frac{\partial c_i}{\partial t} + k_{G,i}c_i\frac{\partial \theta_g}{\partial t} = \theta_g k_{G,i}\frac{\partial c_i}{\partial t} + k_{G,i}c_i\frac{\partial \theta_g}{\partial t} \tag{8-15}$$

where $k_{G,i} = \partial c_{G,i}/\partial c_i$ is the linear volatilization.

SATURATED POROUS MEDIA

In the case of transport in a saturated porous medium, $\theta_l = \varepsilon_p$, and the governing equations are

$$\frac{\partial}{\partial t}(\varepsilon_p c_i) + \frac{\partial}{\partial t}(\rho c_{P,i}) + \mathbf{u}\cdot\nabla c_i = \nabla\cdot[(D_{D,i} + D_{e,i})\nabla c_i] + R_i + S_i \tag{8-16}$$

Convection in Porous Media

Convection (also called advection) describes the movement of a species, such as a pollutant, with the bulk fluid velocity. The velocity field **u** corresponds to a superficial volume average over a unit volume of the porous medium, including both pores and matrix. This velocity is sometimes called *Darcy velocity*, and defined as volume flow

rates per unit cross section of the medium. This definition makes the velocity field continuous across the boundaries between porous regions and regions with free flow.

	The velocity field to be used in the Model Inputs section on the physics interface can, for example, be prescribed using the velocity field from a Darcy's Law or a Brinkman Equations interface.

The average linear fluid velocities $\mathbf{u}_a$, provides an estimate of the fluid velocity within the pores:

$$\mathbf{u}_a = \frac{\mathbf{u}}{\varepsilon_p} \quad \text{Saturated}$$

$$\mathbf{u}_a = \frac{\mathbf{u}}{\theta_l} \quad \text{Unsaturated}$$

where ε_p is the porosity and $\theta_l = s\varepsilon_p$ the liquid volume fraction, and s the saturation, a dimensionless number between 0 and 1.

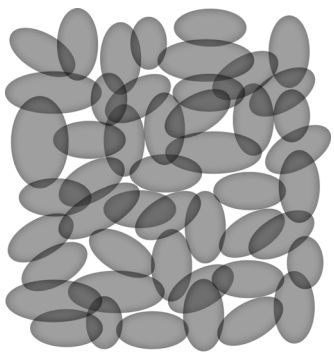


Figure 8-2: A block of a porous medium consisting of solids and the pore space between the solid grains. The average linear velocity describes how fast the fluid moves within the pores. The Darcy velocity attributes this flow over the entire fluid-solid face.

MATERIAL BALANCE FORMULATION

The Transport of Diluted Species interface in porous media includes two formulations of the material balance. The conservative formulation of the species equations in Equation 8-13 is written as:

$$\frac{\partial}{\partial t}(\theta_l c_i) + \frac{\partial}{\partial t}(\rho c_{P,i}) + \frac{\partial}{\partial t}(\theta_g c_{G,i}) + \nabla \cdot \mathbf{u} c_i = \nabla \cdot [(D_{D,i} + D_{e,i})\nabla c_i] + R_i + S_i \tag{8-17}$$

If the conservative formulation is expanded using the chain rule, then one of the terms from the convection part, $c_i \nabla \cdot \mathbf{u}$, would equal zero for an incompressible fluid and would result in the nonconservative formulation described in Equation 8-13.

When using the nonconservative formulation, which is the default, the fluid is assumed incompressible and divergence free: $\nabla \cdot \mathbf{u} = 0$. The nonconservative formulation improves the stability of systems coupled to a momentum equation (fluid flow equation).

	To switch between the two formulations, click the **Show** button ( ) and select **Advanced Physics Options**. In the section **Advanced Settings** select either **Nonconservative** (the default) or **Conservative**. The conservative formulation should be used for compressible flow.

Diffusion in Porous Media

The effective diffusion in porous media, D_e, depends on the structure of the porous material and the phases involved. Dependent on whether the transport of diluted species occurs in free flow or in saturated or unsaturated porous media, the effective diffusivity is defined as:

$$D_e = D_F \qquad \text{Free Flow}$$

$$D_e = \frac{\varepsilon_p}{\tau_L} D_L \qquad \text{Saturated Porous Media}$$

$$D_e = \frac{\theta_l}{\tau_L} D_L \qquad \text{Unsaturated Porous Media}$$

$$D_e = \frac{\theta_l}{\tau_L} D_L + \frac{\theta_g}{\tau_G} k_G D_G \qquad \text{Unsaturated with Volatilization}$$

Here D_F, D_L, and D_G are the single-phase diffusion coefficients for the species diluted in a fluid, a pure liquid, and a gas phase, respectively (SI unit: m^2/s), and τ_F, τ_L, and τ_G are the corresponding tortuosity factors (dimensionless).

The tortuosity factor accounts for the reduced diffusivity due to the fact that the solid grains impede Brownian motion. The interface provides predefined expressions to

compute the tortuosity factors in partially saturated porous media according to the Millington and Quirk model (Ref. 3):

$$\tau_L = \theta_l^{-7/3}\varepsilon_p^{\ 2}\ ,\ \tau_G = \theta_g^{-7/3}\varepsilon_p^{\ 2}$$

and Bruggeman model

$$\tau_L = \theta_l^{-5/2}\varepsilon_p^{\ 2}\ ,\ \tau_G = \theta_g^{-5/2}\varepsilon_p^{\ 2}$$

For saturated porous media $\theta_l = \varepsilon_p$. The fluid tortuosity for the Millington and Quirk model is

$$\tau_L = \varepsilon_p^{\ -1/3}$$

and for the Bruggeman model the tortuosity is defined as

$$\tau_L = \varepsilon_p^{\ -1/2}$$

User defined expressions for the tortuosity factor can also be applied.

Dispersion

The contribution of dispersion to the mixing of species typically overshadows the contribution from molecular diffusion, except when the fluid velocity is very low.

The spreading of mass, as a fluid travel through a porous medium is caused by several contributing effects. Local variations in fluid velocity lead to mechanical mixing referred to as dispersion occurs because the fluid in the pore space flows around solid particles, so the velocity field varies within pore channels. The spreading in the direction parallel to the flow, or *longitudinal dispersivity*, typically exceeds the *transverse dispersivity* from up to an order of magnitude. Being driven by the concentration gradient alone, molecular diffusion rate is low relative to the mechanical dispersion, except at very low fluid velocities.

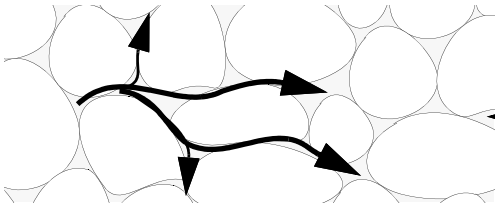


Figure 8-3: Spreading of fluid around solid particles in a porous medium.

The dispersion is controlled through the dispersion tensor D_{D}. The tensor components can either be given by user-defined values or expressions or derived from the directional dispersivities.

Using the longitudinal and transverse dispersivities in 2D, the dispersivity tensor components are (Ref. 5):

$$D_{\mathrm{D}ii} = \alpha_{\mathrm{L}}\frac{u_i^2}{|\mathbf{u}|} + \alpha_{\mathrm{T}}\frac{u_j^2}{|\mathbf{u}|}$$

$$D_{\mathrm{D}ij} = D_{\mathrm{D}ji} = (\alpha_{\mathrm{L}} - \alpha_{\mathrm{T}})\frac{u_i u_j}{|\mathbf{u}|}$$

In these equations, $D_{\mathrm{D}ii}$ (SI unit: m^2/s) are the principal components of the dispersivity tensor, and $D_{\mathrm{D}ji}$ and $D_{\mathrm{D}ji}$ are the cross terms. The parameters α_{L} and α_{T} (SI unit: m) specify the longitudinal and transverse dispersivities; and u_i (SI unit: m/s) stands for the velocity field components.

In order to facilitate modeling of stratified porous media in 3D, the tensor formulation by Burnett and Frind (Ref. 4) can be used. Consider a transverse isotropic media, where the strata are piled up in the z direction, the dispersivity tensor components are:

$$
\begin{aligned}
D_{\mathrm{L}xx} &= \alpha_1 \frac{u^2}{|\mathbf{u}|} + \alpha_2 \frac{v^2}{|\mathbf{u}|} + \alpha_3 \frac{w^2}{|\mathbf{u}|} \\
D_{\mathrm{L}yy} &= \alpha_1 \frac{v^2}{|\mathbf{u}|} + \alpha_2 \frac{u^2}{|\mathbf{u}|} + \alpha_3 \frac{w^2}{|\mathbf{u}|} \\
D_{\mathrm{L}zz} &= \alpha_1 \frac{w^2}{|\mathbf{u}|} + \alpha_3 \frac{u^2}{|\mathbf{u}|} + \alpha_3 \frac{v^2}{|\mathbf{u}|} \\
D_{\mathrm{L}xy} &= D_{\mathrm{L}yx} = (\alpha_1 - \alpha_2) \frac{uv}{|\mathbf{u}|} \\
D_{\mathrm{L}xz} &= D_{\mathrm{L}zx} = (\alpha_1 - \alpha_3) \frac{uw}{|\mathbf{u}|} \\
D_{\mathrm{L}yz} &= D_{\mathrm{L}zy} = (\alpha_1 - \alpha_3) \frac{vw}{|\mathbf{u}|}
\end{aligned}
\tag{8-18}
$$

In Equation 8-18 the fluid velocities u, v, and w correspond to the components of the velocity field $\mathbf{u}$ in the x, y, and z directions, respectively, and α_1 (SI unit: m) is the longitudinal dispersivity. If z is the vertical axis, α_2 and α_3 are the dispersivities in the transverse horizontal and transverse vertical directions, respectively (SI unit: m). Setting $\alpha_2 = \alpha_3$ gives the expressions for isotropic media shown in Bear (Ref. 5 and Ref. 6).

Adsorption

As species travel through a porous medium they typically attach to (adsorb), and detach (desorb) from the solid phase, which slows chemical transport through the porous medium. Adsorption and desorption respectively reduces or increases species concentrations in the fluid. The adsorption properties vary between chemicals, so a plume containing multiple species can separate into components (Ref. 7). The Adsorption feature includes four predefined and one user-defined relationships to predict the solid concentrations, $c_{\mathrm{P}i}$ from the concentration in the liquid phase, c_i:

$$c_P = c_{Pmax}\frac{K_L c}{1 + K_L c} \qquad \text{Langmuir}$$

$$c_P = K_F\left(\frac{c}{c_{ref}}\right)^N \qquad \text{Freundlich}$$

$$c_P = c_{Pmax}\frac{b_T c}{(1 + (b_T c)^{N_T})^{1/N_T}} \qquad \text{Toth} \qquad (8\text{-}19)$$

$$c_P = \frac{K_B c_0 c}{(c_S - c)\left(1 + (K_B - 1)\frac{c}{c_S}\right)} \qquad \text{BET}$$

The above equations contains the following parameters:

- Freundlich (Ref. 8)
  - Freundlich constant K_F (SI unit:·mol/kg), Freundlich exponent N_F (dimensionless), and reference concentration c_{ref} (SI unit: mol/m^3).
- Langmuir (Ref. 9)
  - Langmuir constant K_L (SI unit: m^3/mol), and adsorption maximum c_{Pmax} (SI unit: mol/kg).
- Toth (Ref. 10)
  - Toth constant b_T (SI unit: m^3/mol), Toth exponent N_T (dimensionless), and adsorption maximum c_{Pmax} (SI unit: mol/kg).
- BET (Brunauer–Emmett–Teller, Ref. 11)
  - BET constant K_B (dimensionless), the monolayer adsorption capacity c_0 (SI unit: mol/kg) and the saturation concentration, c_S (SI unit: mol/m^3).

These predefined expressions are adsorption isotherms that describe the amount of species sorbed to the solid. Applying the isotherms, as defined in the Adsorption section above, assumes that adsorption is at equilibrium locally. This implies that the species phase transfer, between the fluid and the solid phase (within the porous medium), is much faster than the transport within the fluid phase.

Using a Species Source feature, arbitrary expressions can be entered to define, for example, nonequilibrium and temperature-dependent adsorption laws, in the manner of Fetter (Ref. 12), or Bear and Verruijt (Ref. 13).

The retardation factor, RF, describes how adsorption slows the solute velocity, $\mathbf{u}_c$, relative to the average linear velocity of the fluid, $\mathbf{u}_a$, as in

$$\mathrm{RF} = 1 + \frac{\rho_b}{\theta}\frac{\partial c_P}{\partial c} = \frac{\mathbf{u}_a}{\mathbf{u}_c}$$

If the contaminant moves at the average linear velocity of the fluid for $\mathrm{RF} = 1$. For $\mathrm{RF} > 1$, the contaminant velocity is lower than the fluid velocity owing to residence time on solids.

Reactions

Chemical reactions of all types influence species transport in porous media. Examples include biodegradation, radioactive decay, transformation to tracked products, temperature- and pressure-dependent functions, exothermic reactions, and endothermic reactions. The reactions represent change in species concentration per unit volume porous medium per time. Reaction terms are used on the right-hand side of the governing equation to represent these processes. For reactions in a fluid phase, multiply the expression by the fluid volume fraction θ. Similarly, solid phase reaction expressions include the bulk density, ρ_b, and gas phase reactions include the gas volume fraction, a_v.

The following expressions define some common types of reactions:

$R_{Li} = -\theta\frac{\ln 2}{\lambda_{Li}}c_i$	Radioactive decay — liquid
$R_{Pi} = -\rho_b\frac{\ln 2}{\lambda_{Pi}}\left(\frac{\partial c_{Pi}}{\partial c_i}\right)c_i$	Radioactive decay — solid
$R_{Gi} = -\frac{\ln 2}{\lambda_{Gi}}a_v\left(\frac{\partial c_{Gi}}{\partial c}\right)c_i$	Radioactive decay — gas
$R_{Lk} = \theta\zeta_{Li}c_i$	Creation from parent c_{Li} — liquid
$R_{Pk} = \rho_b\zeta_{Pi}\left(\frac{\partial c_{Pi}}{\partial c_i}\right)c_i$	Creation from sorbed parent c_{Pi} — solid
$R_{Gk} = -\zeta a_v\left(\frac{\partial c_{Gi}}{\partial c}\right)c_i$	Reaction — gas

where λ is the chemical half life, ζ is a reaction rate, and the subscripts L, P, and G denote liquid, solid, and gas phases, respectively. In the equations, the reactions either depend on liquid concentration c_i or solid phase concentrations c_{Pi} obtained using the sorption derivative with c_i or gas phase concentration c_{Gi} depending on the gas volume fraction, the volatilization, and the liquid concentration.

Reaction rates can vary with results from other equations in your model, such as temperature. For example, enter the Arrhenius rate law given in Ref. 14:

$$\zeta_T = \zeta_R \exp\left[\frac{E_a(T - T_R)}{R_u T T_R}\right] \tag{8-20}$$

In Equation 8-20, T denotes the current absolute temperature, T_R denotes the reference absolute temperature, E_a is the activation energy, and R_u is the universal gas constant.

Mass Transport in Fractures

When thin fractures occur in porous media, fluid flow tends to move faster along the fracture than in the surrounding media. The transport of chemical species therefore also occur also faster in the direction of the fractures.

The fluid flow in a fracture can be modeled using Darcy's law formulated in a thin sheet of porous medium (a fracture):

$$\mathbf{u} = \frac{\kappa}{\mu}\nabla_t p$$

Here $\mathbf{u}$ is the tangential Darcy velocity, κ is the fracture permeability, μ the fluid's dynamic viscosity, and $\nabla_t p$ is the tangential gradient of the fluid pressure.

The equation to solve for mass transport of species c_i in a thin fracture, embedded in a porous media, is derived from Equation 8-13. The resulting equation is:

$$d_{\mathrm{fr}}\left(\frac{\partial \rho_{\mathrm{b}} c_{\mathrm{P},i}}{\partial t} + \frac{\partial \varepsilon_{\mathrm{p}} c_i}{\partial t} + \nabla_{\mathrm{t}} \cdot (D_{\mathrm{e},i} \nabla_{\mathrm{t}} c_i) + \mathbf{u} \cdot \nabla_{\mathrm{t}} c_i\right) = d_{\mathrm{fr}} R_i + d_{\mathrm{fr}} S_i + n_0 \tag{8-21}$$

Here d_{fr} is the fracture thickness, $c_{\mathrm{P},i}$ the amount of species adsorbed to (or desorbed from) the porous matrix (moles per unit dry weight of the solid), ε_{p} is the fracture porosity, and D_{e} is the effective diffusivity. The first two terms on the right hand side represent source terms from reactions, and n_0 corresponds to out-of plane flux from the adjacent porous domain.

In order to arrive at the tangential differential equation, the gradient is split into the contributions normal and tangential to the fracture:

$$\nabla c_i = \nabla_{\mathrm{n}} c_i + \nabla_{\mathrm{t}} c_i$$

The normal gradient is defined in the direction normal to the boundary representing the fracture and the tangential gradient is defined along the boundary. Assuming that the variations in the normal (thin) direction of the fracture are negligible compared to those in the tangential direction, the gradient is simplified as:

$$\nabla c_i = \nabla_t c_i$$

Using The Transport of Diluted Species in Fractures Interface, the transport along fracture boundaries alone is solved for. In this case the transport in the surrounding porous media neglected and the out-of plane flux n_0 vanishes.

	See Fracture for more information about the boundary feature solving Equation 8-21. See for more information about the physics interface solving the equation on boundaries only.

References

1. R. Codina, "A discontinuity-capturing crosswind-dissipation for the finite element solution of the convection-diffusion equation", *Computer Methods in Applied Mechanics and Engineering*, vol. 110, pp. 325–342, 1993.

2. P.V. Danckwerts, "Continuous flow systems: Distribution of residence times", *Chem. Eng. Sci.*, vol. 2, no. 1, 1953.

3. R.J. Millington and J.M. Quirk, "Permeability of Porous Solids", *Trans. Faraday Soc.*, vol. 57, pp. 1200–1207, 1961.

4. R.D. Burnett and E.O. Frind, "An Alternating Direction Galerkin Technique for Simulation of Groundwater Contaminant Transport in Three Dimensions: 2. Dimensionality Effects", *Water Resour. Res.*, vol. 23, no. 4, pp. 695–705, 1987.

5. J. Bear, *Hydraulics of Groundwater*, McGraw Hill, 1979.

6. J. Bear, *Dynamics of Fluids in Porous Media*, Elsevier Scientific Publishing, 1972.

7. D.M. Mackay, D.L. Freyberg, P.V. Roberts, and J.A. Cherry, "A Natural Gradient Experiment on Solute Transport in a Sand Aquifer: 1. Approach and Overview of Plume Movement", *Water Resour. Res.*, vol. 22, no. 13, pp. 2017–2030, 1986.

8. H.M.F. Freundlich, "Über die Adsorption in Lösungen" (in German), *Z. Phys. Chem.*, vol 57, pp. 385–470, 1906

9. I. Langmuir, "The Constitution and Fundamental Properties of Solids and Liquids, Part I Solids", *J. Amer. Chem. Soc.*, vol. 38, pp. 2221–2295, 1916.

10. J. Toth, "State equation of the solid gas interface layer", *Acta Chem. Acad. Hung.* vol. 69, pp. 311–317, 1971.

11. S. Brunauer, P.H. Emmett, E. Teller, "Adsorption of gases in multimolecular layers", *J. Am. Chem. Soc.*, vol. 60 (2), pp. 309–319, 1938.

12. C.W. Fetter, *Contaminant Hydrogeology*, Prentice Hall, 1999.

13. J. Bear and A. Verruijt, *Modeling Groundwater Flow and Pollution*, D. Reidel Publishing, 1994.

14. I. Langmuir, "Chemical Reactions at Low Temperatures", *J. Amer. Chem. Soc.*, vol. 37, 1915.

15. J.M. Coulson and J.F. Richardson, *Chemical Engineering, vol. 2*, 4th ed., Pergamon Press, Oxford, U.K., 1991.

16. J.M. Coulson and J.F. Richardson, *Chemical Engineering, vol. 1*, 4th ed., Pergamon Press, Oxford, U.K., 1991.

17. D.E Rosner, *Transport Processes in Chemically Reacting Flow Systems*, ISBN-13: 978-1483130262, Butterworth–Heinemann, 1986.

18. R.B. Bird, W.E. Stewart, and E.N. Lightfoot, *Transport Phenomena*, 2nd ed., John Wiley & Sons, Inc., 2007.

9

Glossary

This Glossary of Terms contains finite element modeling terms specific to the Microfluidics Module and its applications. For mathematical terms as well as geometry and CAD terms specific to the COMSOL Multiphysics® software and its documentation, see the glossary in the *COMSOL Multiphysics Reference Manual*. To find references in the documentation set where you can find more information about a given term, see the index.

Glossary of Terms

absorption (gas) Uptake of a gas into the bulk of a liquid. Gas absorption takes place, for example, in the liquid of a scrubber tower where an up-streaming gas is washed by a down-going flow of a scrubber solution.

adsorption (molecule) Attachment of a molecule or atom to a solid surface. Adsorption involves a chemical bond between the adsorbed species and the surface.

ALE See *arbitrary Lagrangian-Eulerian method*.

arbitrary Lagrangian-Eulerian (ALE) method A technique to formulate equations in a mixed kinematical description. An ALE referential coordinate system is typically a mix between the material (Lagrangian) and spatial (Eulerian) coordinate systems.

biosensor A general term for sensor devices that either detect biological substances or use antibodies, enzymes, or other biological molecules in their operation. Biosensors are a subcategory of chemical sensors.

Bond number A dimensionless number given by the ratio of surface tension forces to body forces (usually gravity) for a two-phase flow. It is also known as the Eötvös number, Eo. At high Bond numbers surface tension has a minimal effect on the flow; at low Bond numbers, surface tension dominates. The Bond number, Bo, is given by:

$$\mathrm{Bo} = \frac{\rho g L^2}{\sigma}$$

where ρ is the density, g is the body force acceleration, L is the characteristic length, and σ is the surface tension coefficient. The density can refer to a density difference when considering buoyancy.

Brinkman equations A set of equations extending Darcy's law in order to include the transport of momentum through shear in porous media flow.

capillary number A dimensionless number given by the ratio of viscous forces to surface tension for a two phase flow. At low capillary numbers flow in porous media is dominated by surface tension. The capillary number, Ca, is given by

$$\mathrm{Ca} = \frac{\mu v}{\sigma}$$

where μ is the viscosity, v is the characteristic velocity of the problem, and σ is the surface tension coefficient.

continuum flow Fluid flow which is well described by approximating the liquid as a continuum with the Navier–Stokes equations.

convection Transport of molecules or heat due to the movement of the surrounding medium.

creeping flow Models the Navier–Stokes equations without the contribution of the inertia term. This is often referred to as *Stokes flow* and is appropriate for use when viscous flow is dominant, such as in very small channels or microfluidic applications.

crosswind diffusion A numerical technique for stabilization of the numeric solution to a convection-dominated PDE by artificially adding diffusion perpendicular to the direction of the streamlines.

Darcy's Law Equation that gives the velocity vector as proportional to the pressure gradient. Often used to describe flow in porous media.

Debye layer See *electric double layer*.

dielectrophoresis (DEP) Migration of polarizable particles in an electrolyte in a nonuniform applied electric field.

diffusion Transport of material resulting from the random motion of molecules in the presence of a concentration gradient.

Dukhin number A dimensionless number given by the ratio of the surface conductivity contribution to the fluid bulk electric conductivity contribution in electrokinetic phenomena. The Dukhin number, Du, is given by

$$\mathrm{Du} = \frac{K^{\sigma}}{K^{B}}$$

where K^{σ} is the surface conductivity and K^{B} is the bulk conductivity. For low Dukhin numbers, surface conductivities can be neglected when modeling electrokinetic flows.

electric double layer (EDL) Sometimes referred to as the Debye layer. At the contact of a solid and a polar fluid (such as water), the solid acquires an electric charge. This charge attracts ions within the fluid, and a narrow fluid layer of opposite charge, the Stern layer, forms on the boundary. In addition, adjacent to the Stern layer, a wider layer with the same charge as in the Stern layer forms in the fluid. Together, the Stern layer and the wider layer (called the diffuse or Gouy–Chapman layer) form the electric double layer. Due to the close distance between the charges, the Stern layer is fixed on the surface, but the more distant diffuse layer can move.

electrohydrodynamics A general term describing phenomena that involve the interaction between solid surfaces, ionic solutions, and applied electric and magnetic fields. It is frequently used in microfluidic devices to manipulate fluids and move particles for sample handling and chemical separation.

electrokinetics Study of the motion of charged particles under an applied electric field in moving substances such as water.

electrokinetic flow Transport of fluid or charged particles within a fluid by means of electric fields. See also *electroosmosis, electrophoresis, electrothermal flow*, and *dielectrophoresis.*

electrolyte A solution that can carry an electric current through the motion of ions.

electroosmosis Fluid flow in a narrow channel produced by the movement of the *electric double layer* (EDL) along the channel boundary under the influence of an applied electric field. Also, fluid flow through a membrane under the influence of an applied electric field. See also *electric double layer.*

electroosmotic flow See *electroosmosis.*

electrophoresis Migration of charged electrolyte ions or particles in an applied electric field.

electrothermal effects These effects occur in a conductive fluid where the temperature is modified by Joule heating from an AC electric field. This creates variations in conductivity and permittivity and thus Coulomb and dielectric body forces.

electrothermal flow Fluid flow resulting from an applied nonuniform AC electric field on a fluid. The Joule heating changes the fluid's electrical properties locally, and that effect, together with the power gradient of the AC electric field, results in fluid motion.

electrowetting The *electrowetting effect* describes the change in solid-electrolyte contact angle that occurs when a potential difference is applied between the solid and the electrolyte.

electrowetting-on-dielectric (EWOD) A form of *electrowetting* in which a thin insulating layer separates the conducting solid surface from the electrolyte.

Eötvös number See *Bond number*.

Eulerian frame A frame of reference with its coordinate axes fixed in space.

Fick's laws The first law relates the concentration gradients to the diffusive flux of low concentration solute diluted in a solvent. The second law introduces the first law into a differential material balance for the solute.

fluid-structure interaction (FSI) When a flow affects the deformation of a solid object and vice versa.

free molecular flow The flow of gas molecules through a geometry which is much smaller than the mean free path (Knudsen number, $\mathrm{Kn} > 10$). In the free molecular flow regime the gas molecules collide with the walls of the geometry much more frequently than they collide with themselves.

fully developed laminar flow Laminar flow along a channel or pipe that has velocity components only in the main direction of the flow. The velocity profile perpendicular to the flow does not change downstream in the flow.

Gouy–Chapman layer See *electric double layer (EDL)*.

Hagen–Poiseuille equation See *Poiseuille's law*.

Helmholtz–Smoluchowski equation Gives the velocity of a parallel electroosmotic flow for an applied electric field.

intrinsic volume averages The physical properties of the fluid, such as density, viscosity, and pressure.

Knudsen number A dimensionless number that provides a measure of how rarefied a gas flow is, in other words, the mean free path of the gas molecules compared to the length scale of the flow. The following equation defines the Knudsen number Kn in terms of the mean free path λ of the molecules and a length scale L characteristic of the flow:

$$\mathrm{Kn} = \frac{\lambda}{L}$$

Knudsen layer A layer of rarefied fluid flow that occurs within a few mean free paths of the walls in a gas flow. The continuum Navier–Stokes equations break down in this layer.

Lagrangian frame A frame of reference with its coordinate axes fixed in a reference configuration of a deforming material. As the material deforms, the Lagrangian frame deforms with it.

Laplace number The Laplace number, La, (also known as the Surataman number, Su) relates the inertial and surface tension forces to the viscous forces. It is used to describe the breakup of liquid jets and sheets: at high Laplace and low Reynolds numbers the Rayleigh Instability occurs, at low Laplace and high Reynolds numbers atomization occurs. The Laplace number is given by

$$\mathrm{La} = \frac{\rho\sigma L}{\mu^2}$$

where ρ is the fluid density, σ is the surface tension coefficient, L is the characteristic length scale of the problem, and μ is the viscosity. The Laplace number is directly related to the Ohnesorge number, Oh, through the equation $\mathrm{La} = 1/\mathrm{Oh}^2$.

Mach number Ratio of the convective speed, v, to the speed of sound in the medium, a. The Mach number, Ma, is defined by the equation

$$\mathrm{Ma} = \frac{v}{a}$$

magnetohydrodynamics Fluid-flow phenomena involving magnetic fields.

magnetophoresis Migration of magnetic or paramagnetic particles suspended in a fluid as a result of an applied magnetic field. The field must be nonuniform in the case of paramagnetic particles.

Marangoni effect Fluid flow parallel to an interface induced by surface tension gradients.

Marangoni number Ratio of thermal surface tension forces to viscous forces. The Marangoni number, Mg, is given by:

$$\mathrm{Mg} = \frac{d\sigma}{dT}\frac{L\Delta T}{\mu\alpha}$$

where σ is the surface tension coefficient, T is the absolute temperature (ΔT is the characteristic temperature difference), L is the characteristic length, and α is the thermal diffusivity ($\alpha = \kappa/(\rho c_p)$), where c_p is the heat capacity at constant pressure, κ is the thermal conductivity, and ρ is the density of the fluid.

microfluidics Study of the behavior of fluids at the microscale. Also refers to MEMS fluidic devices.

migration The transport of charged species in an electrolyte due to the electric force imposed by the electric field.

mobility The relation between the drift velocity of a molecule within a fluid and the applied electric field.

Newtonian flow Flow characterized by a constant viscosity or a viscosity that is independent of the shear rate in the fluid.

Nernst–Planck equation Flow equation that describes the flux of an ion through diffusion, convection, and migration in an electric field. The equation is valid for diluted electrolytes.

Ohnesorge number A dimensionless number relating the inertial and surface tension forces to the viscous forces. Used to describe the breakup of liquid jets and sheets: at low Ohnesorge and Reynolds numbers the Rayleigh instability occurs; at high Ohnesorge and Reynolds numbers, atomization occurs. The Ohnesorge number, Oh, is given by:

$$\mathrm{Oh} = \frac{\mu}{\sqrt{\rho\sigma L}}$$

where ρ is the fluid density, σ is the surface tension coefficient, L is the characteristic length scale of the problem, and μ is the viscosity. The Ohnesorge number is directly related to the Laplace number, La, through the equation $\mathrm{Oh} = 1/\mathrm{La}^{1/2}$.

Peclet number A dimensionless number describing the ratio of convection to diffusion in a fluid flow. The Peclet number, Pe, can be used to describe concentration diffusion or heat diffusion. It is given by

$$\mathrm{Pe} = \frac{vL}{D}$$

where v is the convective velocity, L is the flow length scale, and D is the diffusion constant.

Poiseuille's law Equation that relates the mass rate of flow in a tube as proportional to the pressure difference per unit length and to the fourth power of the tube radius. The law is valid for fully developed laminar flow.

Reynolds number A dimensionless number classifying how laminar or turbulent a flow is. The *Reynolds number* Re is a measure of the relative magnitude of the flow's viscous and inertial forces. It is defined by the following equation where ρ is the fluid density, μ is the dynamic viscosity, ν is its kinematic viscosity, v is a velocity characteristic to the flow, and L is a length scale characteristic to the flow.

$$\mathrm{Re} = \frac{\rho v L}{\mu} = \frac{vL}{\nu}$$

slip flow Fluid flow that occurs when the *Knudsen number*, Kn, is in the range $0.01 < \mathrm{Kn} < 0.1$. As a result of rarefaction effects in the *Knudsen layer* the no slip boundary condition fails. The flow outside the Knudsen layer can be represented by the continuum Navier–Stokes equations provided that an appropriate slip boundary condition is used for the fluid flow and the correct temperature jump boundary condition is applied at the interface.

streamline diffusion A numerical technique for stabilization of the numeric solution to a convection-dominated PDE by artificially adding diffusion in the direction of the streamlines.

Stern layer A layer of immobile ions and associated solvent molecules present at the solid-liquid interface in an electric double layer (EDL).

Stokes flow See *creeping flow*.

superficial volume averages The flow velocities, which correspond to a unit volume of the medium including both pores and matrix. They are sometimes called Darcy velocities, defined as volume flow rates per unit cross section of the medium.

surface tension Surface tension is a property of the surface of a liquid that allows it to resist an external force. Equivalently it can be through of as the energy per unit area of the liquid surface. It is caused by asymmetries in the cohesive forces between molecules at the surface of the liquid.

Surataman number See *Laplace number*.

transitional flow Fluid flow that occurs when the *Knudsen number*, Kn, is in the range $0.1 < \mathrm{Kn} < 10$. In this regime the flow is so rarefied that continuum equations break down completely. However collisions between the molecules are still important, so free molecular flow is not applicable.

Weber number A dimensionless number describing the ratio of inertial forces to surface tension forces. The Weber number is given by

$$\mathrm{We} = \frac{\rho v^2 L}{\sigma}$$

where ρ is the density of the fluid, v is the characteristic velocity of the flow, L is the characteristic length scale, and σ is the surface tension coefficient.

zeta potential The potential of at the interface between the electric double layer and a solid surface in an electrolyte.

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